Benzene C-H Bond Activation in Carboxylic Acids Catalyzed by O-donor Ir(III) Complexes: An Experimental and Density Functional Study

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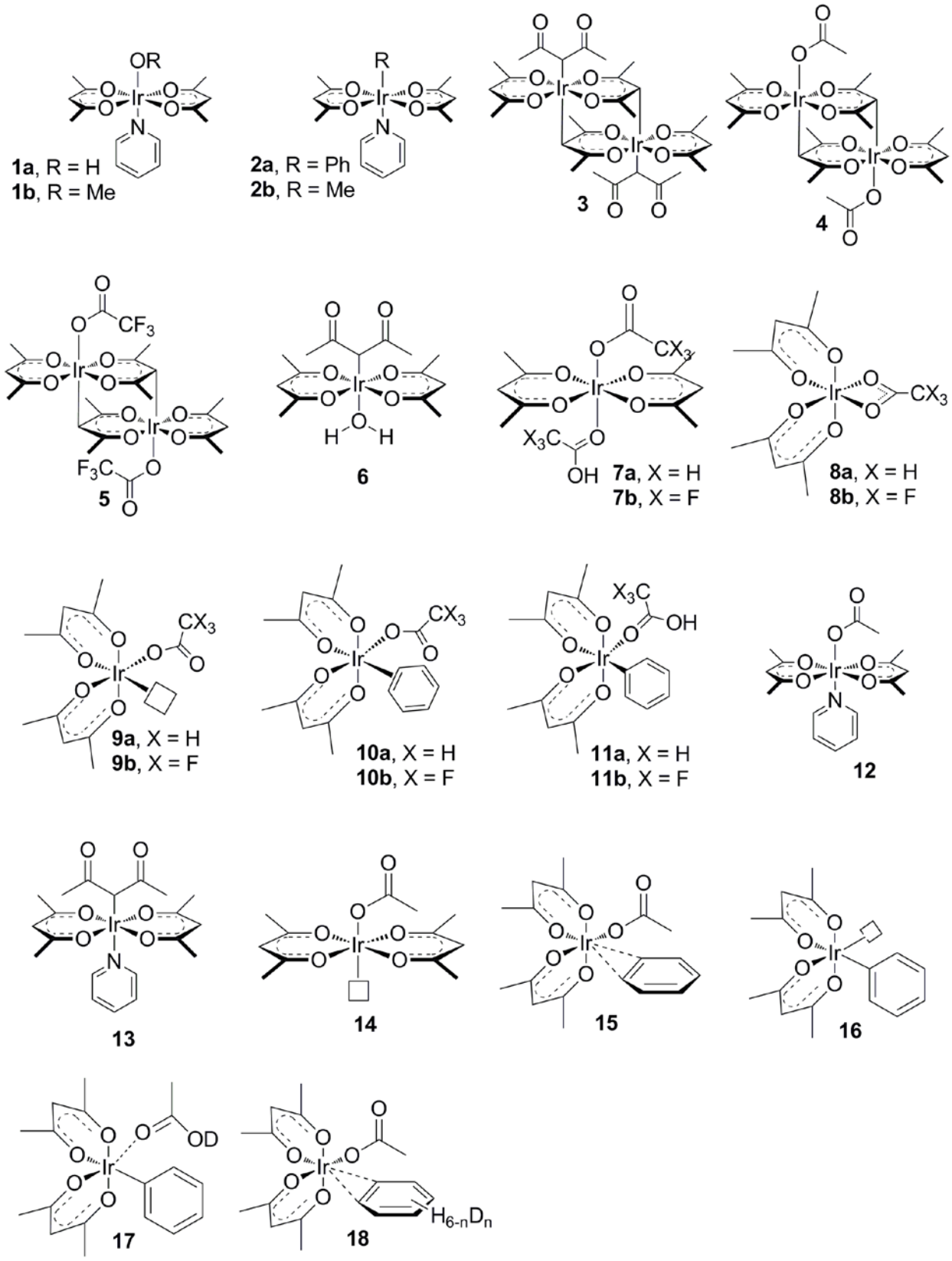
General Procedures: All manipulations were carried out using an argon filled MBraun glovebox and standard Schlenk techniques. Benzene was used directly from an MBraun solvent purification system after passing through an activated molecular sieves column or via distillation over Na/benzophenone. Reagent-grade chemicals and solvents were purchased from Sigma Aldrich and $IrCl_3 \cdot H_2O$ from Pressure Chemical. Deuterated solvents were purchased from Cambridge Isotope or Sigma Aldrich and used as is. Deuterated acetic acid and deuterated trifluoroacetic acid were degassed before use by several freeze-pump-thaw cycles and stored under argon. Elemental analyses were performed by Columbia Analytical Services; Tucson, Arizona. Fast Atom Bombardment (FAB+) or Electrospray Ionization (ESI) mass spectroscopy was performed at UC Riverside Mass Spec Facility; Riverside, California or at the University of Florida Mass Spec Facility; Gainesville, Florida. Flash

chromatography was performed on a Teledyne Isco CombiFlash Rf with prepacked Teledyne Isco alumina or silica columns using HPLC or better grade solvents. Liquid phase organic products were analyzed with a Shimadzu GC-MS QP5000 (ver. 2) equipped with cross-linked methyl silicone gum capillary column, DB5, or a Shimadzu GC-MS QP2010S equipped with cross-linked methyl silicone gum capillary column, RTX-5. Gas measurements were performed using a GasPro column. The retention times of the products were confirmed by known standards. NMR spectra were obtained on a Bruker AC-250 (250.134 MHz for ^{1}H and 62.902 MHz for ^{13}C), a Varian Mercury 400 (400.151 MHz for ^{1}H and 100.631 MHz for ^{13}C), or Bruker Digital Avance III 400 (400.132 MHz for ^{1}H, 100.623 MHz for ^{13}C, and 376.461 MHz for ^{19}F) spectrometer. Chemical shifts are given in ppm relative to residual solvent proton resonances or to a stated internal or external standard. IR Spectra were recorded on a Perkin-Elmer Spectrum One FTIR Spectrometer. Complexes **3**, **6**, and **12** were prepared according to previously reported procedures.[1]

Scheme S 1. Iridium Compounds **1-18**.



General Procedure for H/D Exchange: A 4 mL schlenk flask with a resealable Teflon valve and a magnetic stir bar was charged with 1.0 mL ($1.75x10^{-2}$ mol) of CD_3COOD, 0.5 mol % of catalyst (unless otherwise mentioned) and 0.10 mL (1.12 mmol) benzene-H_6. The flask was degassed (freeze, pump, thaw 3 cycles) and placed under an argon atmosphere. The flask was heated for 30 min in a well stirred oil bath maintained at 130 °C (unless otherwise mentioned). The liquid phase was sampled and analyzed by GC-MS. The percent deuterium incorporation into benzene was determined by deconvoluting the mass fragmentation pattern for benzene using a Microsoft Excel program.[2] An important assumption is built into the program is that there are no isotope effects on the fragmentation pattern of benzene. The parent ion peak of benzene is relatively stable towards fragmentation and can be used to quantify the exchange reactions. The mass fragmentation pattern from m/z of 78 to 84 was analyzed for each reaction and compared to control reactions not containing catalyst. The results obtained by this method are accurate within ± 5 % of deuterium incorporation or loss. Background H.D. exchange between solvent and substrate does not occur in acetic acid and in trifluoroacetic acid, background reactions were subtracted from reported values.

Water Inhibition Study: A 4 mL schlenk flask with a resealable-Teflon valve and a magnetic stir bar was charged with 1.0 mL ($1.75x10^{-2}$ mol) CD_3COOD, 5.0 mg (5.56 μmol, 0.50 mol %) of **4,** 0.1 mL (1.12 mmol) benzene-H_6 and 0 – 100 μL (0 – 4.6mM) D_2O. The flask was degassed (freeze, pump, thaw 3 cycles) and placed under an argon atmosphere. The flask was heated for 30 min in a well stirred oil bath maintained at constant temperature (120 °C). The liquid phase was sampled and analyzed by GC-MS. The percent deuterium incorporation into benzene was determined by deconvoluting the mass fragmentation pattern for benzene using a Microsoft Excel program**.**

Mercury Drop Test using 4: A 4 mL schlenk flask with a Teflon valve and a magnetic stir bar was charged with 1.0 mL ($1.75x10^{-2}$ mol) CD_3COOD 5.0 mg (5.56 μmol, 0.50 mol %) of **4** and 0.10 mL (1.12 mmol) benzene-H_6. Two drops of elemental mercury were added to the reaction flask. The flask was degassed (freeze, pump, thaw 3 cycles) and placed under an argon atmosphere. Control reactions were set up to include a reaction with catalyst 5.0 mg (5.56 μmol, 0.50 mol %) of **2** and with two drops Hg^0 and no catalyst. Reaction flasks were then placed in an oil bath (150 °C) for 1 hour. The liquid phase was sampled and analyzed by GC-MS. The percent deuterium incorporation into benzene was determined by deconvoluting the mass fragmentation pattern for benzene using a Microsoft Excel program.

Comparing Solvent Effects on Rate and Mechanism: A 4 mL schlenk flask with a resealable-Teflon valve and a magnetic stir bar was charged with 1 mL ($1.75x10^{-2}$ mol) CD_3COOD or 1.0 mL (0.013 mol) of CF_3COOD, 5 mg (5.56 μmol, 0.5 mol %) of **4** and 0.10 mL (1.12 mmol) benzene-H_6. The flask was degassed (freeze, pump, thaw 3 cycles) and placed under an argon atmosphere. The flask was heated for 120 min in a well stirred oil bath maintained at constant temperature (120 °C). The liquid phase was sampled and analyzed by GC-MS. The percent deuterium incorporation into benzene was determined by deconvoluting the mass fragmentation pattern for benzene using a Microsoft Excel program**.**

Order in Catalyst: A stock solution of ~5 mM in catalyst **4** or **5** was prepared and then diluted by a series of serial dilutions to give lower concentrations of ~2.5 mM and ~1.25 mM. An aliquot (1 mL) was transferred to a 4 mL schlenk flask with a resealable-Teflon valve and 0.1 mL benzene-H_6 added

the mixture. The flask was placed under an argon atmosphere. Over the course of reaction, aliquots of the reaction mixture were monitored by GC-MS over the course of the reaction up to 7.25h. The percent deuterium incorporation into benzene was determined by deconvoluting the mass fragmentation pattern for benzene using a Microsoft Excel program.

Order in Substrate: A stock solution of ~5 mM in catalyst **4** or **5** was prepared. An aliquot (1 mL) was transferred to a 4 mL schlenk flask with a resealable-Teflon valve and 47, 100, or 223 uL of benzene-H_6 added the mixture. The flask was placed under an argon atmosphere. Over the course of reaction, aliquots of the reaction mixture were monitored by GC-MS over the course of the reaction up to 7.25h. The percent deuterium incorporation into benzene was determined by deconvoluting the mass fragmentation pattern for benzene using a Microsoft Excel program.

Stability Tests of 4: A 12 mL schlenk flask with a resealable-Teflon valve was charged with 6 mL (0.105 mol) CD_3COOD or CH_3COOH and 30 mg (33.4 μmol) of **4**. The flask was degassed (freeze, pump, thaw 3 cycles) and placed under an argon atmosphere. Over the course of reaction, 1 mL aliquots of the reaction mixture were taken every 2 hours (T= 0-8 hours) under an argon flow. Aliquots were transferred to a J-young NMR tube and the solvent was removed *in vacuo*. To the dry reaction solid, a premixed internal standard/NMR solvent mixture was added. Internal/NMR solvent mixture was prepared by adding 35 μL (0.55 mmol) dichloromethane to 10 mL (0.12 mol) $CDCl_3$ in a 10 mL volumetric flask. The reaction was monitored by ^1H NMR over a period of 8 hours.

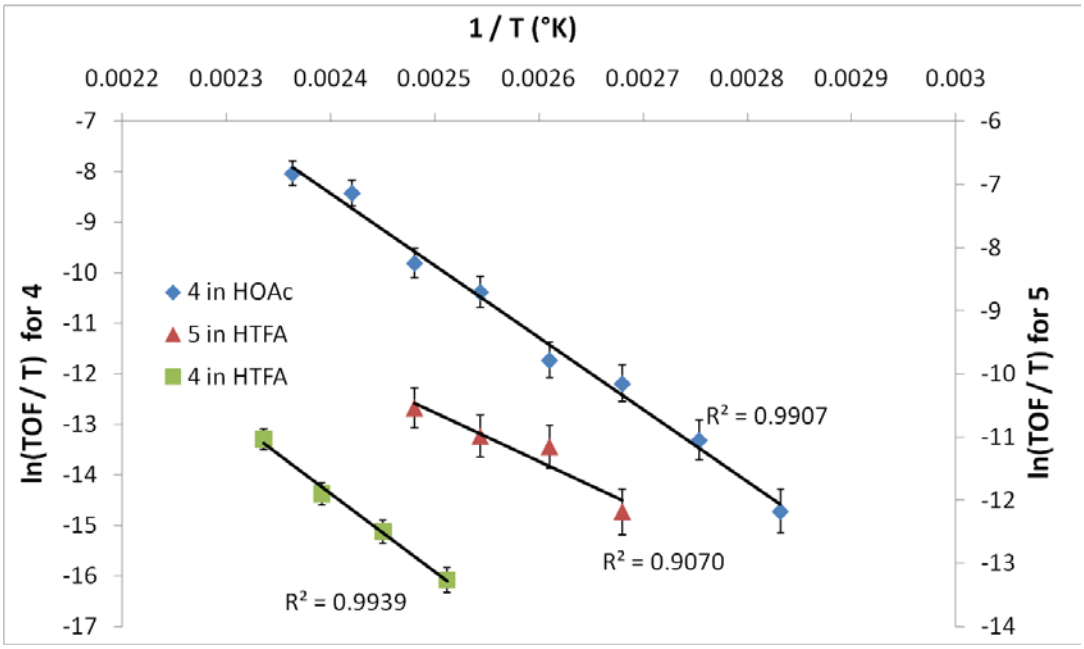


Figure S 1. Eyring plots for **4** in HOAc (♦, $\Delta H^{\ddagger} = \Delta H^{\ddagger} = 28.3 \pm 1.1$ kcal/mol, $\Delta S^{\ddagger} = 3.9 \pm 3.0$ cal K^{-1} mol^{-1}, $R^2 = 0.9907$) and HTFA (■, $\Delta H^{\ddagger} = 21.7 \pm 1.4$ kcal/mol, $R^2 = 0.9939$) and **5** in HTFA (▲,$\Delta H^{\ddagger} = 15.3 \pm 3.5$ kcal/mol, $\Delta S^{\ddagger} = -30.0 \pm 5.1$ cal K^{-1} mol^{-1}, $R^2 = 0.9070$).

Shown in Figure S 3 is the Eyring plot for calculation of the activation parameters of **4** in HOAc and HTFA and **5** in HTFA. Linear regression of these plots gives access t$\Delta S^{\ddagger}$ and $\Delta H^{\ddagger}$. The calculated values experimentally for three the three systems are highlighted in Table S 1 below. One consideration here is important is that when using **4** in HTFA is that the acetate ligand is rapidly substituted off and replaced by TFA. This gives rise to a mix ligand system with multiple active catalysts. Because this system is a mixture we report the activation barriers for relative comparison with the two specific ligand/solvent catalyst systems.

Table S 1. Rate comparison of TOF (130 °C) and experimental enthalpies and entropies of activation for **4** in HOAc and HTFA and **5** in HTFA between 100 - 130 °C.

Catalyst	Solvent	TOF (s^{-1})	$\Delta H^{\ddagger}$ (kcal/mol)	$\Delta S^{\ddagger}$ (cal/K mol)
4	DOAc-D_4	2.62×10^{-3}	28.3 ± 1.1	2.9 ± 3.0
4	DTFA-D_1	6.92×10^{-3}	21.7 ± 1.4	-15.2 ± 1.6
5	DTFA-D_1	1.07×10^{-2}	15.3 ± 3.5	-30.0 ± 5.1

Selectivity of the C-H Bond Activation

Toluene H/D exchange using 4: A 4 mL Schlenk flask with Teflon valve was charged with 1 mL (1.75×10^{-2} mol) CD_3COOD, 5.0 mg (5.56 µmol, 0.60 mol %) of **4,** and 0.10 mL (0.94 mmol) toluene. The flask was degassed (freeze, pump, thaw 3 cycles) and placed under an argon atmosphere. The flask was then placed in a temperature controlled oil bath for 48 hours at 130 °C. Using a 10 mL volumetric flask, an internal standard was prepared using 125 µL (2.13×10^{-3} mol) dichloromethane into 10 mL (0.125 mol) $CDCl_3$. The reaction was sampled under a flow of argon over a 48 hour period and monitored by ^{1}H NMR.

Mesitylene H/D exchange using 4: A J-young NMR tube was charged with 1.0 mL (1.75×10^{-2} mol) CD_3COOD, 5.0 mg (5.56 µmol, 0.80 mol %) of **4,** and 0.1 mL (0.72 mmol) mesitylene. The NMR tube was then freeze pump thawed and backfilled with argon (~1 atm). An external standard was prepared using 0.50 mL (7.8×10^{-3} mol) dichloromethane and 2 mL (2.3×10^{-2} mol) benzene-D_6 and flame sealed in a capillary tube under vacuum. The NMR tubes were placed in a well stirred oil bath maintained at 130 °C. NMR tubes were monitored by ^{1}H NMR over a period of 113 hours and integrated relative to the dichloromethane peak in the external standard.

The selectivity of the C-H bond activation by catalyst **4** was probed by monitoring H/D exchange reactions between deuterated acetic acid and toluene or mesitylene. The H/D exchange reactions were

monitored by ^{1}H NMR and amount of exchange was compared to an internal standard. Toluene was tested for H/D exchange using **4** in acetic acid. Selectivity of toluene deuterium incorporation was observed as the following after 48 hours at 130 °C. The relative percent incorporation observed was ~5% methyl, ~44% ortho/para, and ~69% meta relative to an internal standard as monitored by ^{1}H NMR. H/D exchange reactions were run under similar conditions to the toluene experiment above and mesitylene showed 10% methyl group deuterium incorporation after 110 hours at 130 °C with no deuterium incorporation at the sterically blocked arene positions.

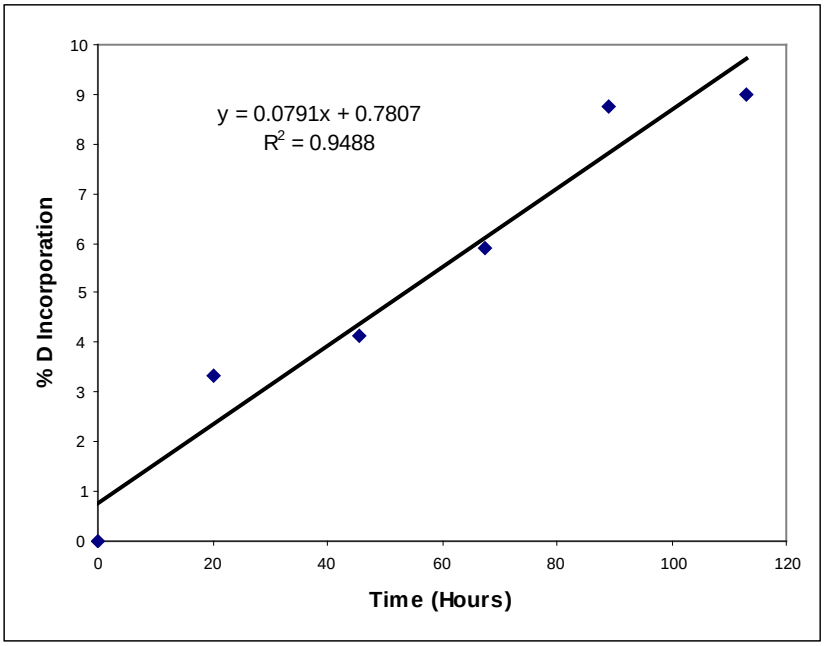


Figure S 2. Mesitylene activation by **4** over a period of 110 hours monitored by ^{1}H NMR.

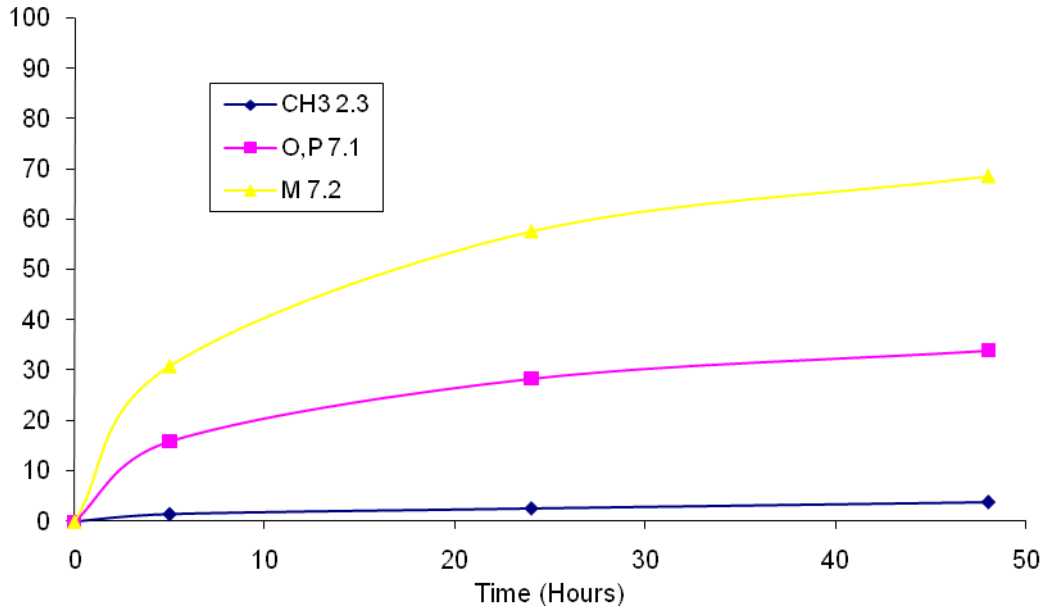
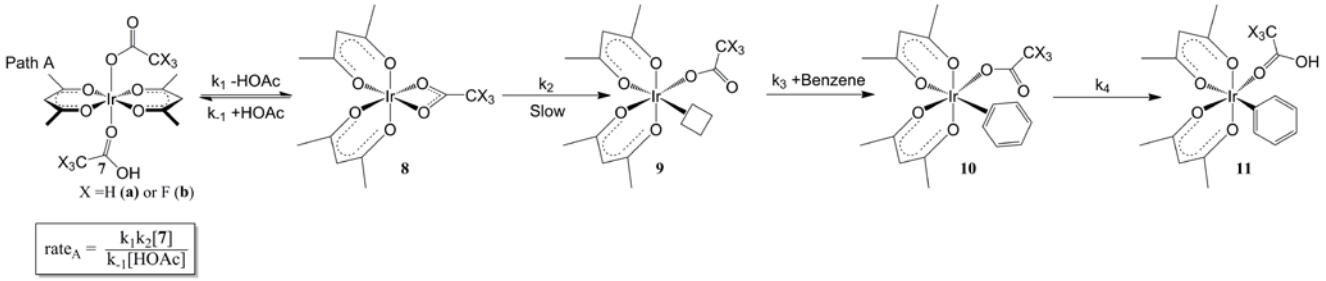
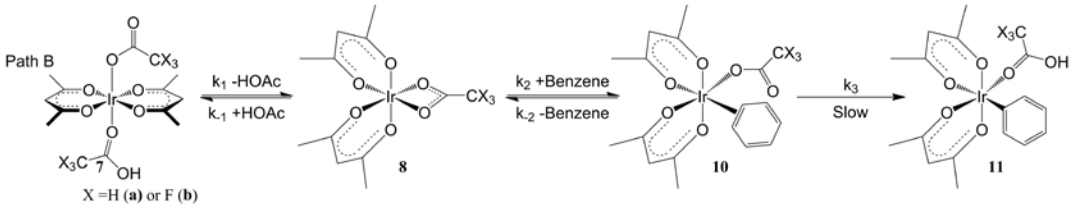


Figure S 3. Plot of H/D exchange over 48 hours between deuterated acetic acid and toluene at 130 °C using **4** as a catalyst.

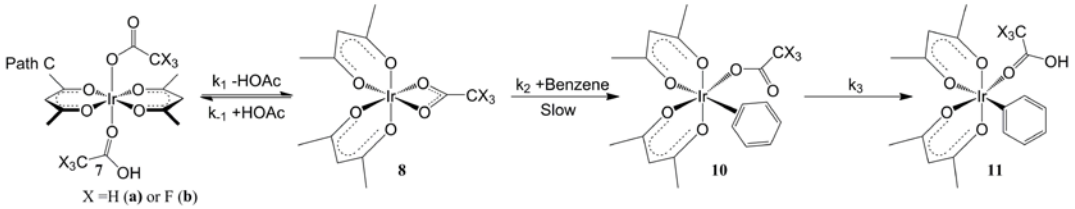
Scheme S 2. Proposed mechanisms for CH activation using **4** and **5** in solution (**7a** and **7b**) where Path A is a associative process in which coordination is rate determining, Path B is an associative process in which cleavage is rate determining, Path C is a dissociative process in which cleavage is rate determining, and Path D is a dissociative process in which coordination is rate determining.



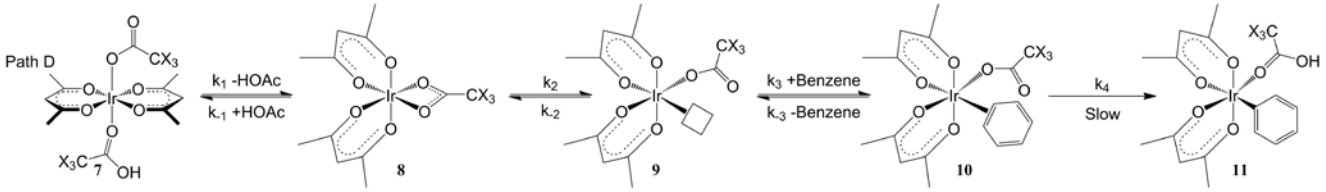
$$rate_A = \frac{k_1 k_2 [7]}{k_{-1}[HOAc]}$$



$$rate_B = \frac{k_1 k_2 k_3 [PhH][7]}{k_{-1}[HOAc](k_3 + k_2)}$$



$$rate_C = \frac{k_1 [PhH][7]}{k_{-1}[HOAc]}$$



$$rate_D = \frac{k_1 k_2 k_3 k_4 [PhH][7]}{k_{-1}[HOAc](k_4 k_{-2} + k_3 k_4 [PhH] + k_{-3} k_{-2})}$$

Table S 2. First order data for **4**.

Time		A_t				-ln(At/Ao)	
(min)	**1.19mM**	**2.38mM**	**4.76mM**		**1.19mM**	**2.38mM**	**4.76mM**
0	1.017213	1.017213	1.017213		0	0	0
60	0.8844	0.973285	0.984589		0.139913	0.044146	0.032598
120	0.766728	0.91771	0.956206		0.28269	0.10294	0.061849
180	0.705679	0.899829	0.942984		0.365662	0.122618	0.075773
240	0.672055	0.826275	0.910687		0.414482	0.207895	0.110622
300	0.627721	0.796327	0.918446		0.482727	0.244812	0.10214
435	0.506122	0.689528	0.818908		0.698044	0.388815	0.216851

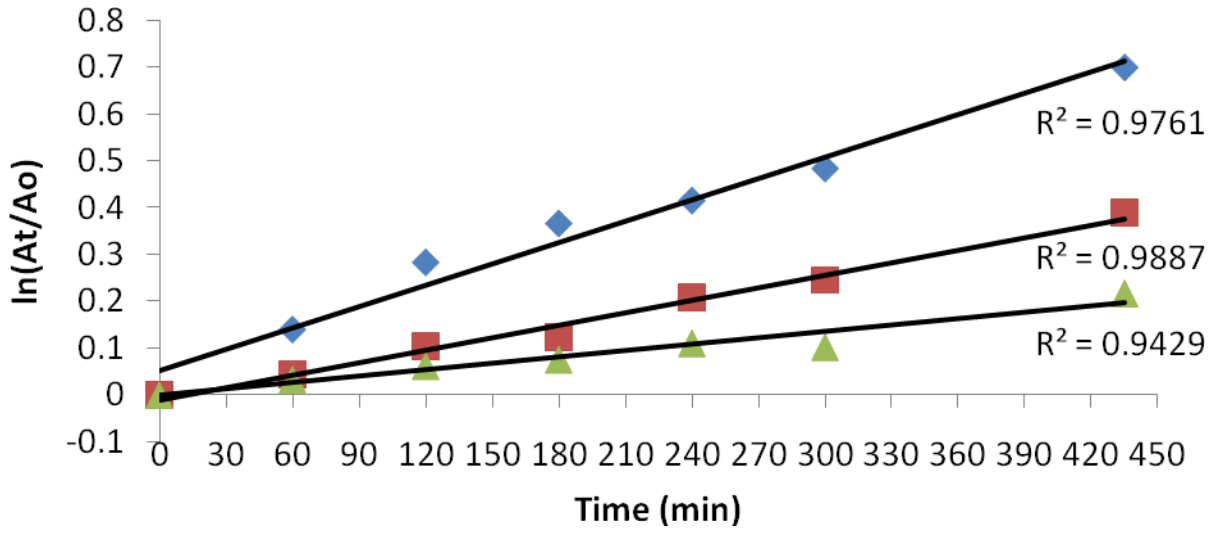


Figure S 4. First order plot for **4** where ♦ = 4.76mM, ■ = 2.38mM, and ▲ = 1.19mM.

Table S 3. Zero and first order data for benzene using **4** where [benzene] = 0.502 M, 1.02 M, or 2.04 M.

		A_t				$\ln(A_t)$	
Time	**0.50M**	**1.02M**	**2.04M**		**0.50M**	**1.02M**	**2.04M**
0	0.502292	1.017213	2.040249		-0.68857	0.017067	0.713072
15	0.49118	0.980538	1.966703		-0.71095	-0.01965	0.676358
30	0.480006	0.93961	1.901163		-0.73396	-0.06229	0.642466
45	0.466347	0.911562	1.837818		-0.76283	-0.0926	0.608579
60	0.442774	0.872922	1.763608		-0.8147	-0.13591	0.567362
75	0.442239	0.840044	1.73666		-0.8159	-0.1743	0.551964
90	0.438347	0.818158	1.684855		-0.82474	-0.2007	0.521679
105	0.425111	0.783312	1.634116		-0.85541	-0.24422	0.491102
120	0.398538	0.748024	1.566996		-0.91995	-0.29032	0.44916
150	0.377416	0.708235	1.473605		-0.97441	-0.34498	0.387712
180	0.355716	0.66609	1.424713		-1.03362	-0.40633	0.35397
210	0.308116	0.596615	1.342105		-1.17728	-0.51648	0.294239
240	0.28837	0.573128	1.253232		-1.24351	-0.55665	0.225726

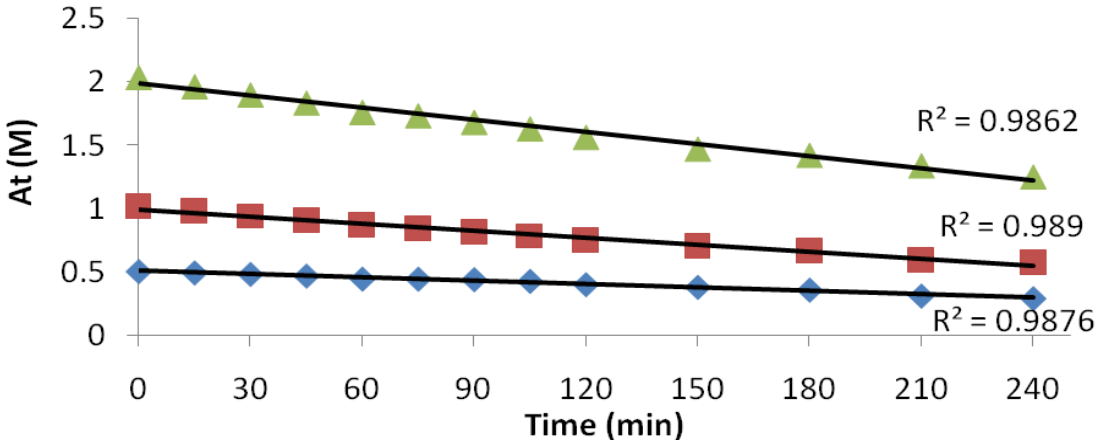


Figure S 5 Zero order plot for benzene using **4** as the catalyst where [benzene] is ♦ = 0.50 M, ■ = 1.02 M, and ▲ = 2.04 M.

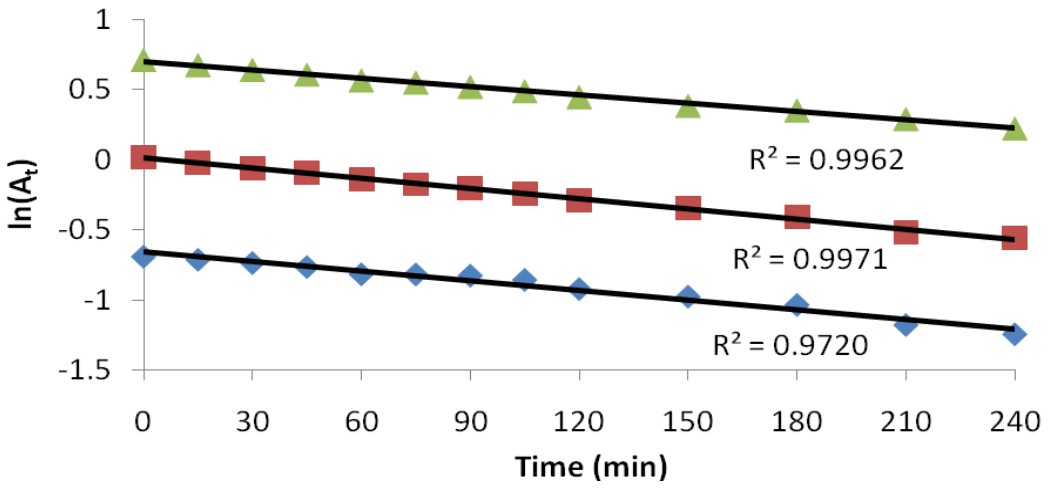


Figure S 6. First order plot for benzene using **4** as the catalyst where [benzene] is ♦ = 0.50 M, ■ = 1.02 M, and ▲ = 2.04 M.

Table S 4. Rate data for **4** by changing [benzene].

TOF (s^{-1})			
Time	**0.50M**	**1.02M**	**2.04M**
15	0.002094	0.007261	0.016188
30	0.0021	0.007681	0.015307
45	0.002258	0.006972	0.014852
60	0.002819	0.007172	0.015297
75	0.002263	0.007015	0.013364
90	0.002008	0.006568	0.013037
105	0.002078	0.006615	0.01277
120	0.002457	0.006693	0.013083
150	0.002366	0.006146	0.012531
180	0.002314	0.005821	0.011345
210	0.002637	0.006002	0.011076
240	0.002542	0.005545	0.010925

Table S 5. First order data for **5** by changing [**5**].

Time		A_t				$\ln(A_t)$	
	4.03 mM	**2.02 mM**	**1.01 mM**		**4.03 mM**	**2.02 mM**	**1.01 mM**
0	1.0172	1.0172	1.0172		0.0171	0.0171	0.0171
15	0.9837	0.9847	0.9902		-0.0165	-0.0154	-0.0098
30	0.8970	0.9023	0.9287		-0.1087	-0.1028	-0.0740
45	0.8569	0.8955	0.9089		-0.1545	-0.1104	-0.0955
60	0.7776	0.7992	0.8443		-0.2515	-0.2242	-0.1693
90	0.6916	0.7555	0.7817		-0.3687	-0.2804	-0.2463
120	0.6040	0.6897	0.7279		-0.5042	-0.3716	-0.3176
150	0.5163	0.6246	0.6653		-0.6610	-0.4707	-0.4076
180	0.4520	0.5614	0.6157		-0.7940	-0.5773	-0.4850

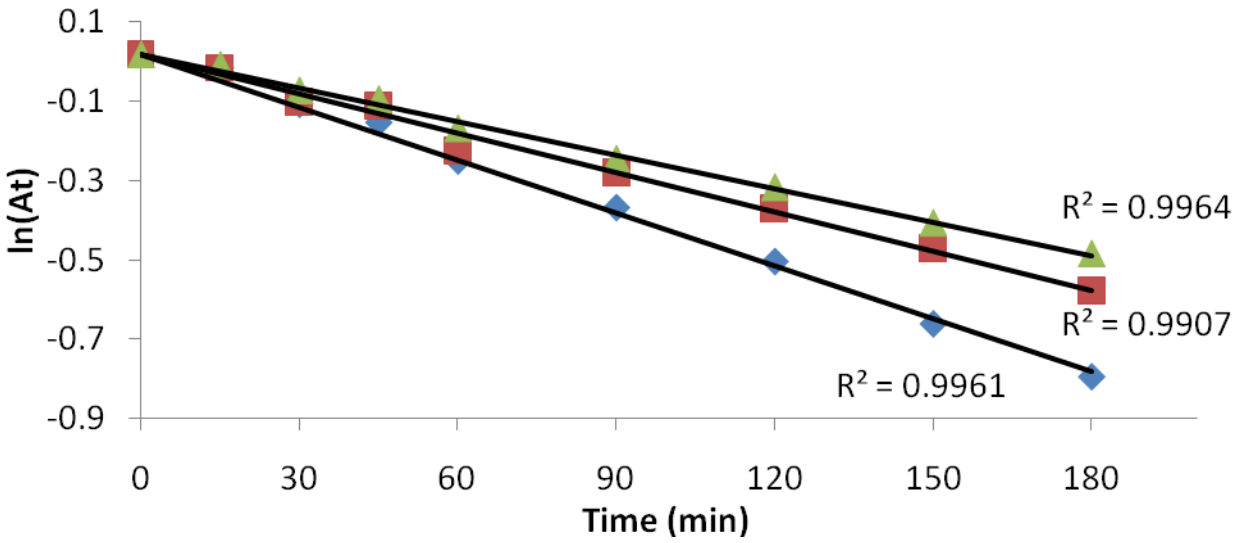


Figure S 7. First order plot for **5** as a catalyst where [**5**] is ♦ = 4.03 mM, ■ = 2.02 mM, and ▲ = 1.01 mM.

Table S 6. First order data for benzene using **5** where [benzene] is changed to be 0.50 M, 1.02 M, and 2.04 M.

		At				ln(At)	
Time	**0.50 M**	**1.02 M**	**2.04 M**		**0.50 M**	**1.02 M**	**2.04 M**
0	0.5022917	1.0172135	2.0402491		-0.68857	0.017067	0.713072
30	0.4345209	0.8705244	1.7959074		-0.83351	-0.13866	0.58551
60	0.3780433	0.7900247	1.606873		-0.97275	-0.23569	0.47429
90	0.3404405	0.729946	1.4731759		-1.07751	-0.31478	0.387421
120	0.3072475	0.6825542	1.4276536		-1.1801	-0.38191	0.356032
150	0.28565	0.6408605	1.3819839		-1.25299	-0.44494	0.32352
180	0.2677279	0.6095611	1.3080601		-1.31778	-0.49502	0.268545
210	0.249985	0.5861945	1.2702508		-1.38635	-0.5341	0.239214
240	0.2343667	0.5575778	1.2023223		-1.45087	-0.58415	0.184255

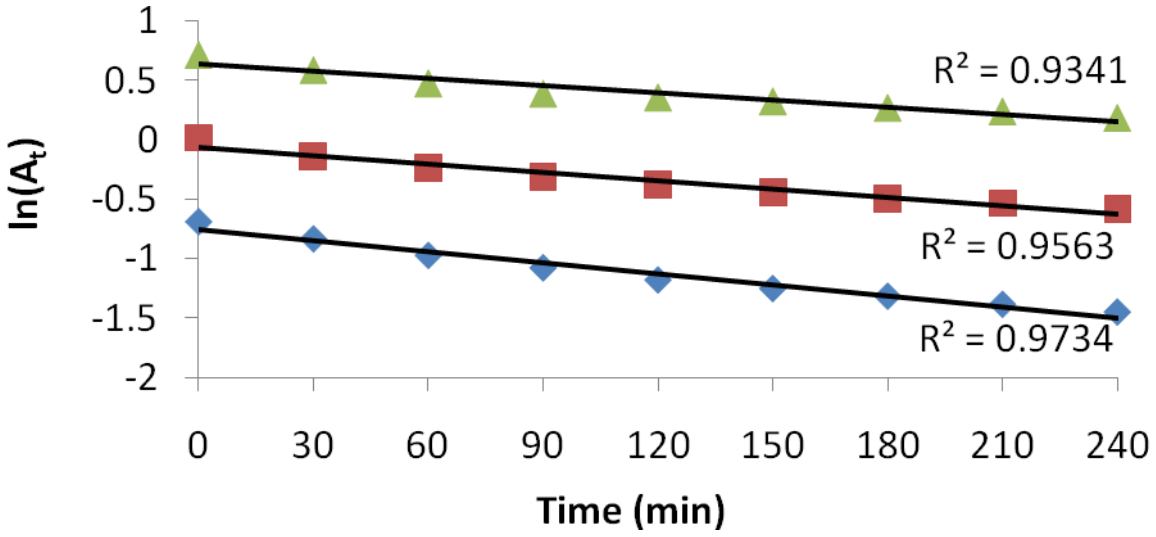


Figure S 8. First order plot for benzene using **5** as the catalyst where ♦ = 0.502 M, ■ = 1.02 M, and ▲ = 2.04 M.

Table S 7. Initial rate data for **5** under H/D exchange conditions while modifying [benzene].

TOF (s-1)		Average	
Time	**0.50 M**	**1.02 M**	**2.04 M**
30	0.009652	0.021948	0.040647
60	0.008847	0.016996	0.036047
90	0.007683	0.014327	0.031445
120	0.006944	0.012518	0.025477
150	0.006462	0.012128	0.021901
180	0.005568	0.010166	0.0203
210	0.005133	0.009213	0.018299
240	0.00477	0.008597	0.017424

Table S 8. Data for comparison between **2** and **12**.

Time	D (M)				Average	Average
	OAc-Ir-Pyr	**OAc-Ir-Pyr**	**Ph-Ir-Pyr**	**Ph-Ir-Pyr**	**OAc-Ir-Pyr**	**Ph-Ir-Pyr**
60	0.02812559	0.03600291	0.02675469	0.0373445	0.03206425	0.03204962
180	0.06813926	0.08529355	0.06297394	0.0878054	0.0767164	0.0753897
300	0.09871681	0.09944413	0.09050193	0.1220351	0.09908047	0.10626853
Time	TOF				Average	Average
	OAc-Ir-Pyr	**OAc-Ir-Pyr**	**Ph-Ir-Pyr**	**Ph-Ir-Pyr**	**OAc-Ir-Pyr**	**Ph-Ir-Pyr**
60	0.00082045	0.00105024	0.00093036	0.0012986	0.00093535	0.00111448
180	0.00066257	0.00082937	0.00072994	0.0010178	0.00074597	0.00087386
300	0.00057594	0.00058018	0.00062941	0.0008487	0.00057806	0.00073907

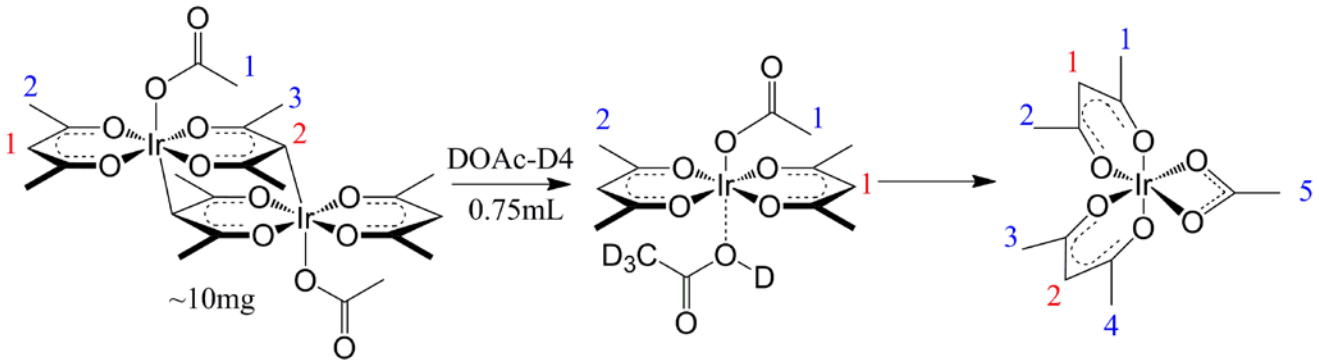
Table S 9. Data for Eyring analysis of **4**.

Temp	Temp K	TOF	1/T	ln(k/T)
80	353.15	0.000143	0.002832	-14.7195
90	363.15	0.0006	0.002754	-13.3134
100	373.15	0.001894	0.00268	-12.1912
110	383.15	0.003092	0.00261	-11.7274
120	393.15	0.012204	0.002544	-10.3802
130	403.15	0.022254	0.00248	-9.80453
140	413.15	0.091222	0.00242	-8.41827
150	423.15	0.137842	0.002363	-8.02937

Table S 10. Data for Eyring analysis of **5**.

Temp	Temp K	TOF	1/T	ln(k/T)
100	373.15	0.006631855	0.00268	-12.1843
110	383.15	0.005479864	0.00261	-11.1551
120	393.15	0.005479864	0.002544	-10.9901
130	403.15	0.005479864	0.00248	-10.5389

Scheme S 3. Conversion of *trans*-$[Ir(acac)_2(OAc)]_2$, **4** to mononuclear-*trans*-$[(acac\text{-}O,O)_2Ir(OAc)(L)]$ where L is a solvent molecule or mononuclear-*cis*-$[(acac\text{-}O,O)_2Ir(\kappa^2\text{-}OAc)]$.



By ^{1}H NMR should see:
3 methyls
2 methines

By ^{1}H NMR should see:
2 methyls
1 methine

By ^{1}H NMR should see:
5 methyls
2 methines

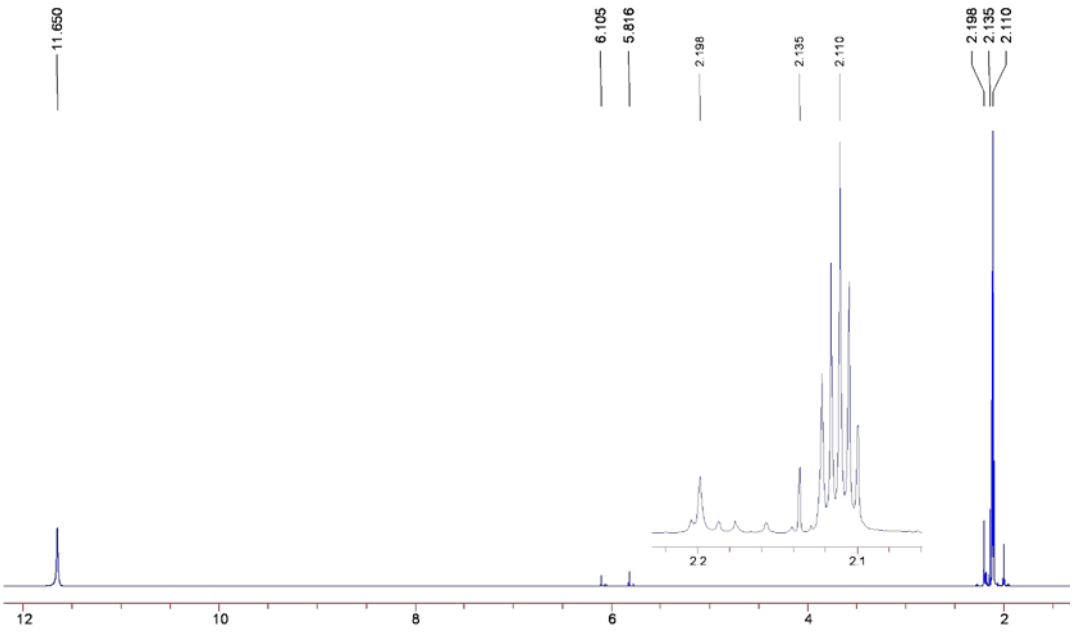


Figure S 9. Initial ^{1}H NMR of **4** at 25 °C in DOAc-D_4.

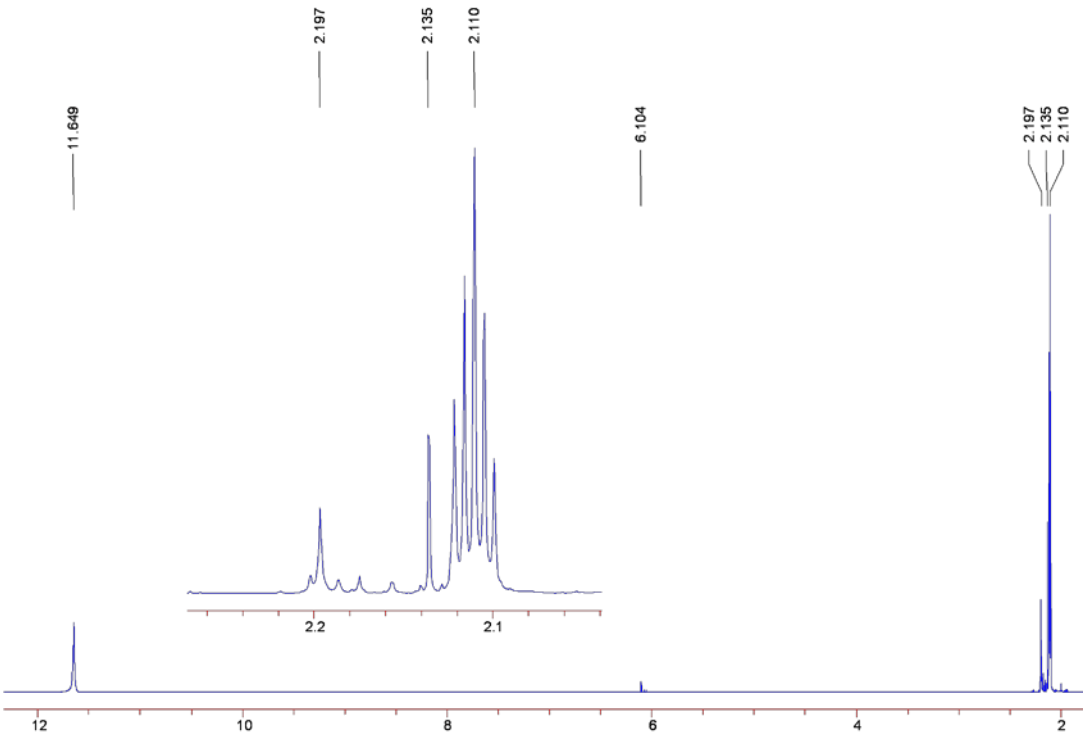


Figure S 10. ^{1}H NMR of **4** at 25 °C in DOAc-D_4 after heating at 100 °C for 20 min**.**

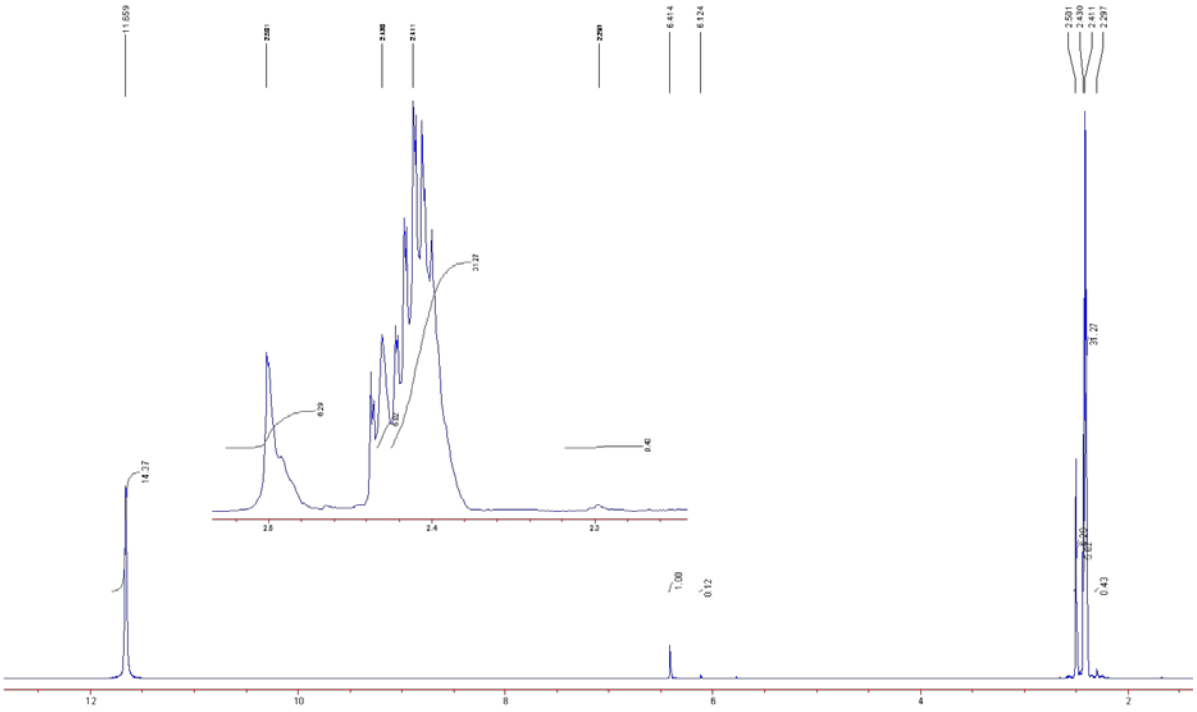


Figure S 11. ^{1}H NMR of **4** at 40 °C in DOAc-D_4.

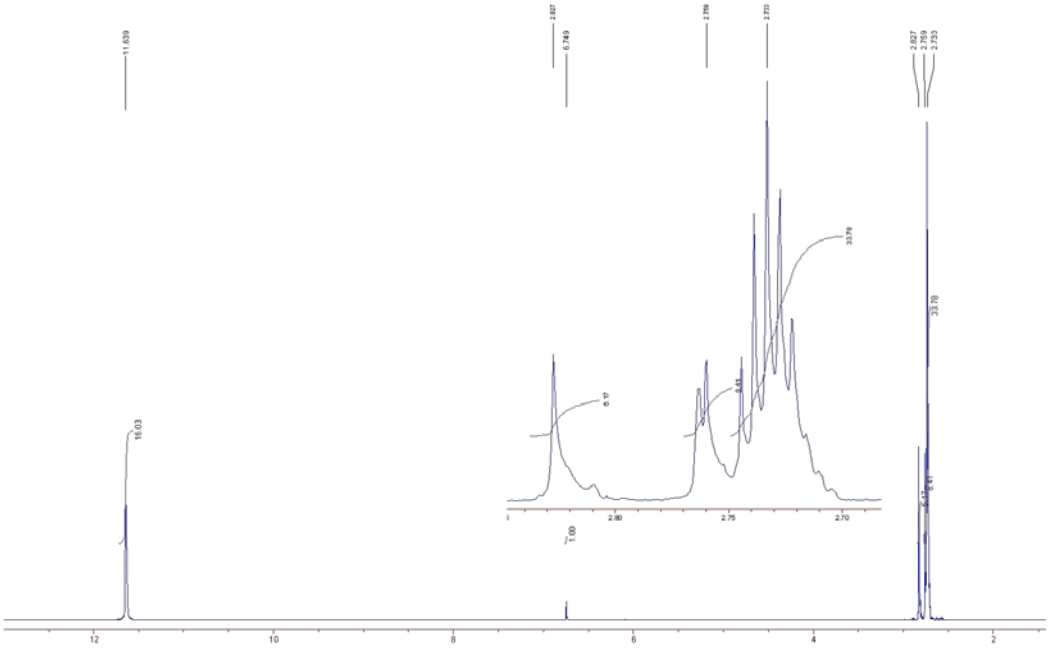


Figure S 12. ^{1}H NMR of **4** at 60 °C in DOAc-D_4.

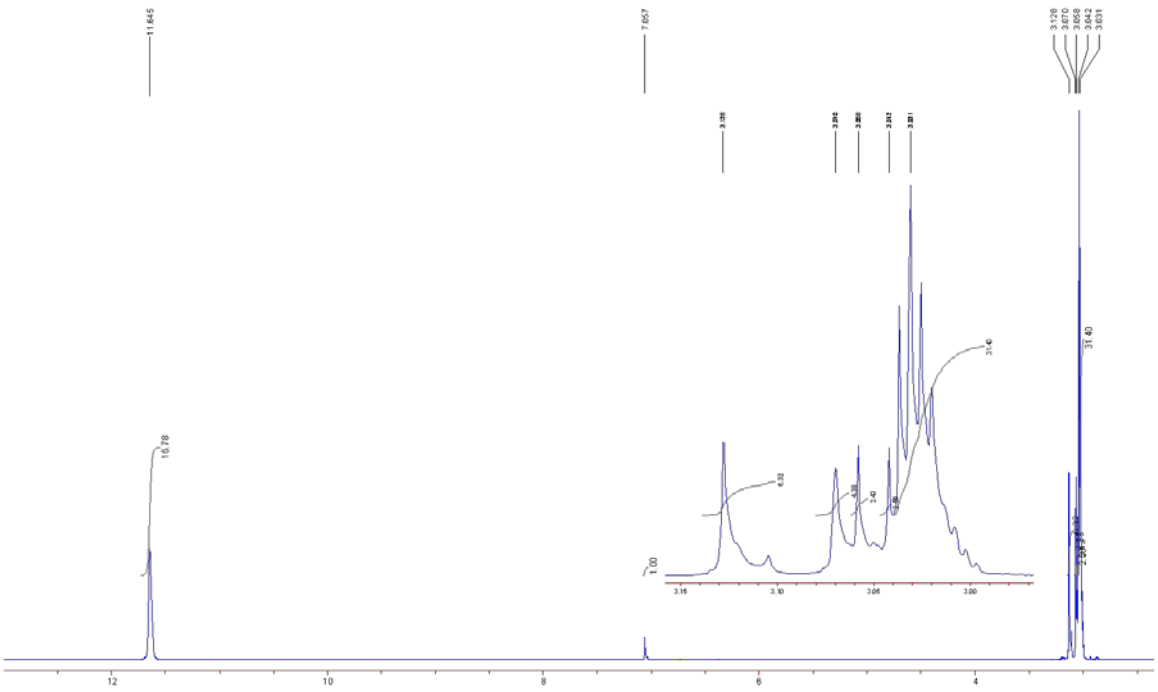


Figure S 13. ^{1}H NMR of **4** at 80 °C in DOAc-D_4.

Table S 11. Data for 1/[CsOAc] inhibition study.

CsOAc (M)	**1/[OAc]**	**TOF (s^{-1})**
0		0.004118
0.020839846	47.985	0.004145
0.096621103	10.34971	0.001852
0.170507829	5.864833	0.001053
0.248183618	4.029275	0.000643

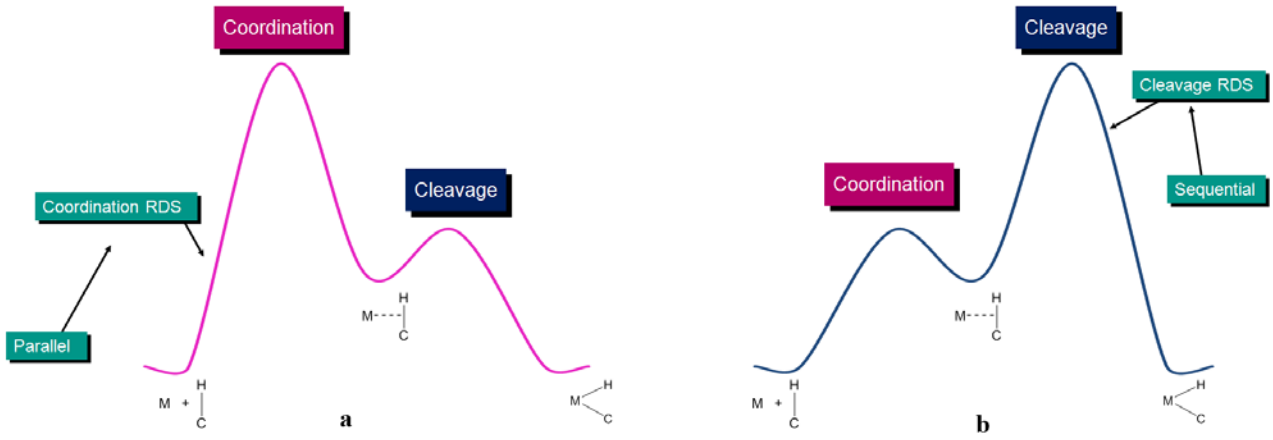
Table S 12. Data for 1/[Pyridine] inhibition study.

Entry	**Eq. of Pyr**	**[Pyr](M)**	**1/[Pyr]**	**TOF (s^{-1})**
1	2.1	0.02033257	49.18219	4.28E-05
2	3.0	0.02904652	34.42753	2.88E-05
3	5.0	0.04841087	20.65652	2.15E-05
4	10.0	0.09682174	10.32826	1.16E-05

Table S 13. Data for H_2O inhibition study.

H_2O Added (uL)	[Water] (mM)	1/L	TOF (s^{-1})	ln(TOF)
0	0.0000	N/A	0.015805	-4.14745
10	0.4979	2.008428	0.009492	-4.65731
25	1.2282	0.814228	0.005305	-5.23905
50	2.4029	0.416161	0.004025	-5.51512
100	4.6056	0.217127	0.001859	-6.28784

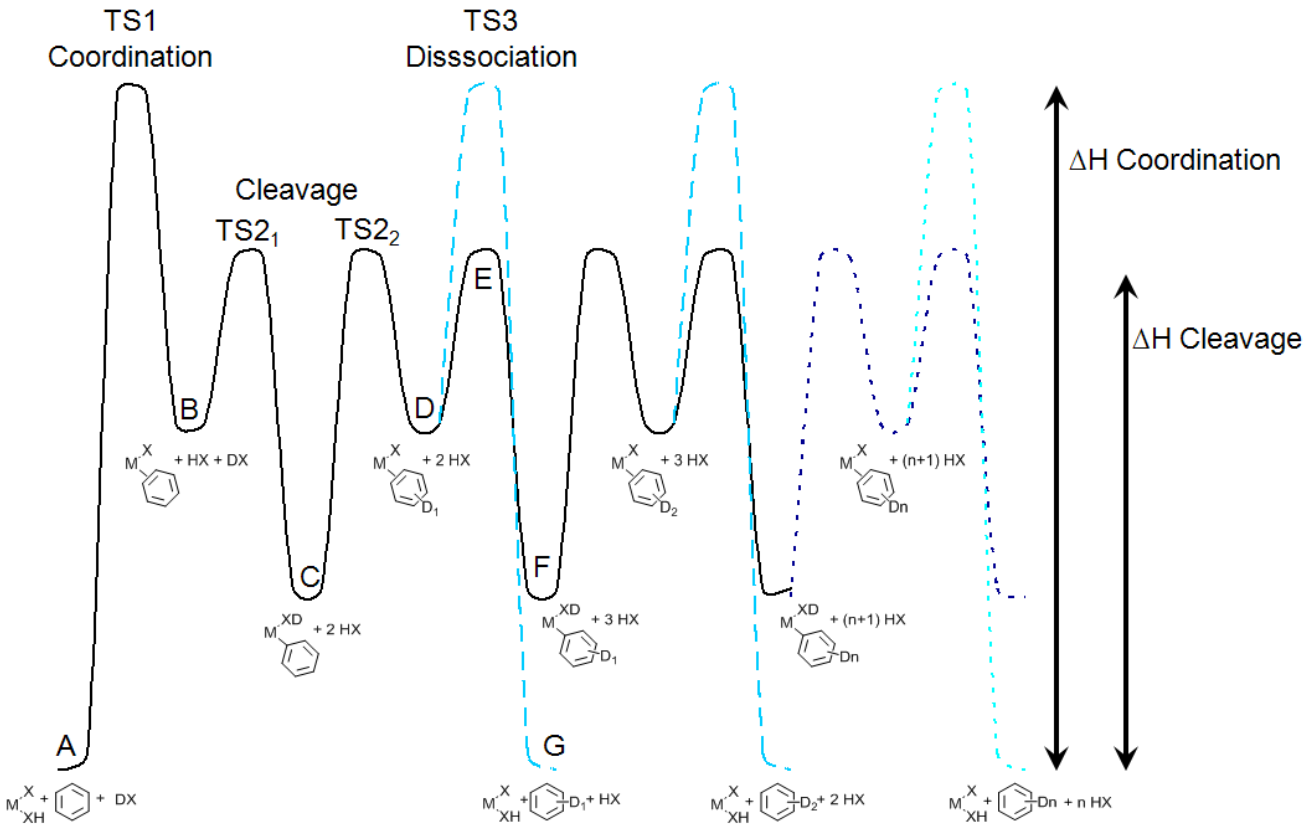
Scheme S 4. Coordination versus cleavage for CH activation.



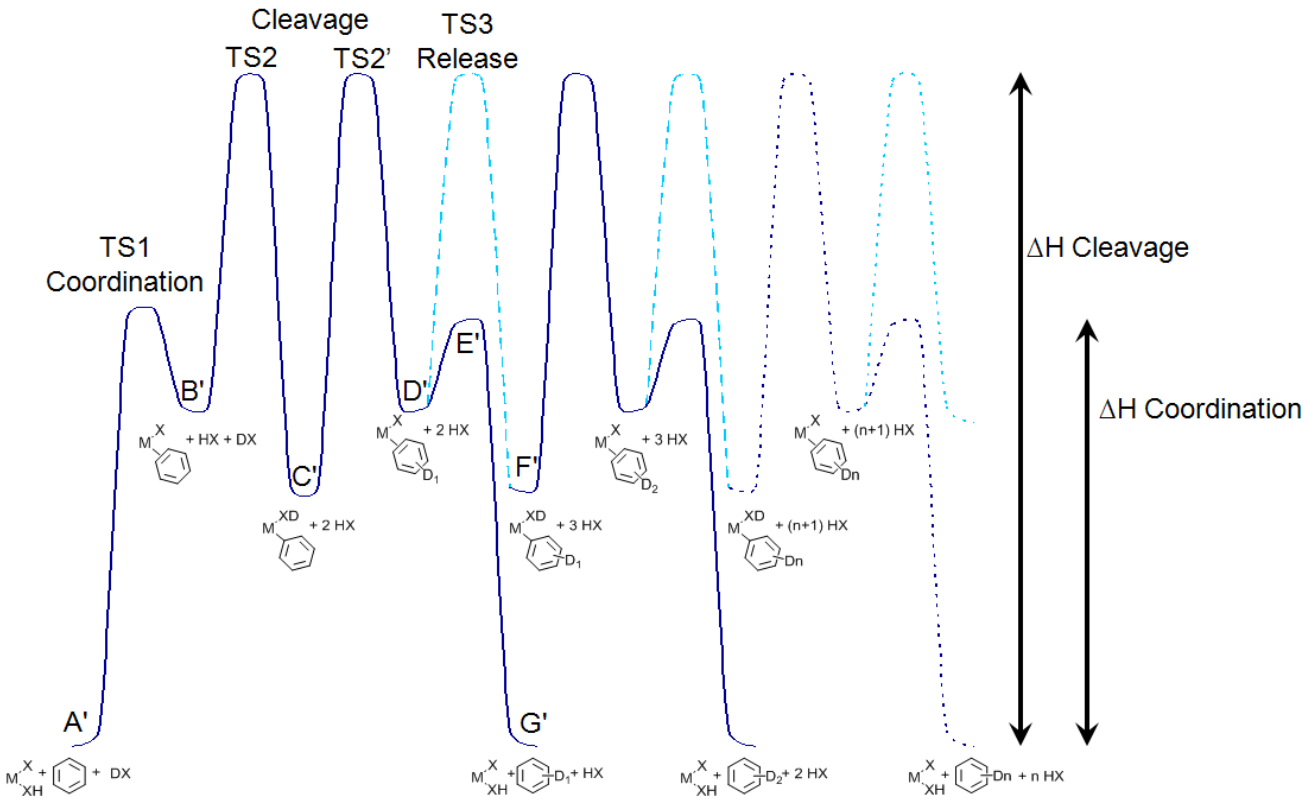
Scheme S 3 shows the possible mechanistic steps when considering CH activation: 1) coordination and 2) cleavage. When coordination is rate determining (**a**), the highest energetic barrier is for the formation of the coordinated alkane or arene complex followed by a fast step of C-H bond cleavage. This situation allows for the occurrence of parallel deuterium incorporation by allowing multiple C-H bond cleavages before the substrate can be released. Contrasting the case when coordination is rate determining is when C-H cleavage is rate determining (**b**). In this case, a rapid pre-equilibrium exists between coordinated and uncoordinated substrate. This then leads to a high energetic barrier for the cleavage of the C-H bond to generate a M-C intermediate. When monitoring H/D reactions in which

cleavage is rate determining a sequential isotopolog formation occurs because when envoking the microscopic reverse reaction from the M-C intermediate to form the alkane or arene complex the rapid equilibrium leads to uncoordinated species.

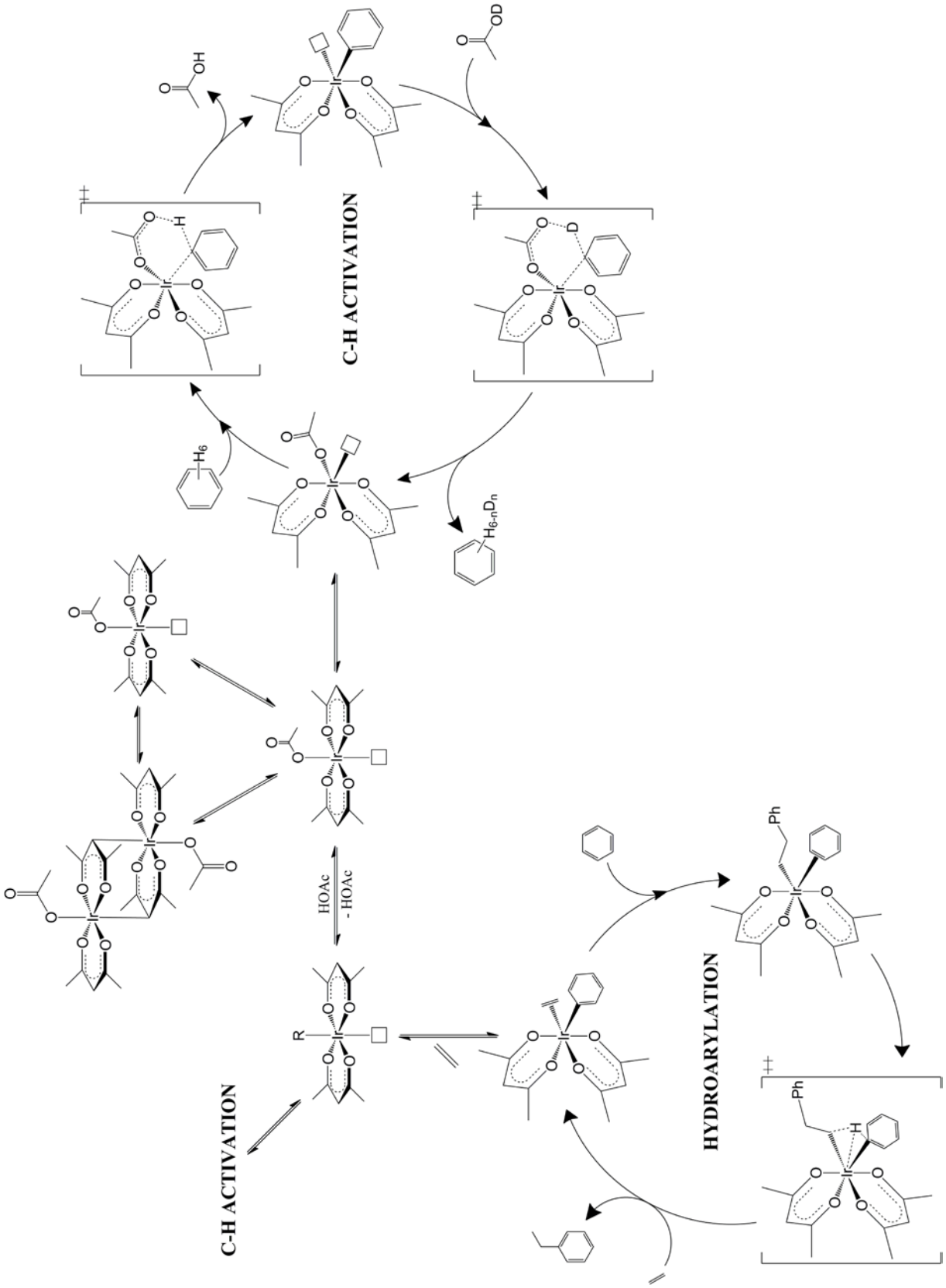
Scheme S 5. Parallel formation relative energy diagram as seen in HOAc.



Scheme S 6. Sequential formation relative energy diagram as seen in HTFA.



Scheme S 7. Overall Catalytic Scheme Showing Inhibition by Hydroarylation



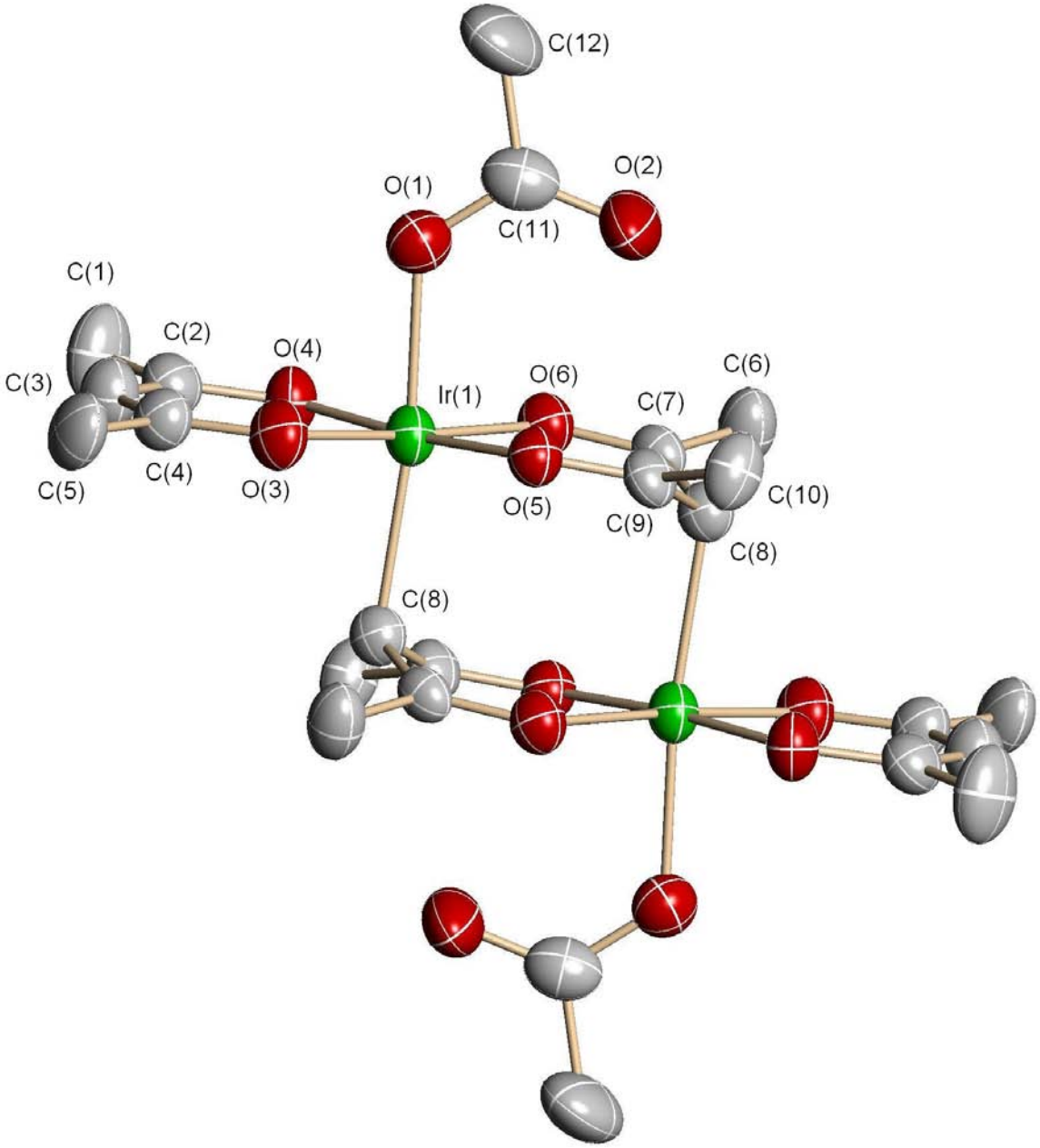


Figure S 14. X-ray crystal structure of **4**.

Table S 14. Crystal data and structure refinement for Ir2O12C24H32.

Identification code	[Ir2O12C24H32]*[2 CHCl3]*H2O	
Empirical formula	C26 H36 Cl6 Ir2 O13	
Formula weight	1153.65	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	P2(1)/m (# 11)	
Unit cell dimensions	a = 7.9845(12) Å	α = 90.0°
	b = 23.481(4) Å	β = 106.231˚
	c = 10.7492(16) Å	γ = 90.0˚
Volume	1935.0(5) Å3	
Z	4	
Density (calculated)	3.960 Mg/m3	
Absorption coefficient	14.680 mm-1	
F(000)	2208	
Crystal size	.12 x .08 x .05 mm3	
Theta range for data collection	1.73 to 24.71°.	
Index ranges	-9<=h<=9, -27<=k<=15, -12<=l<=12	
Reflections collected	9742	
Independent reflections	3398 [R(int) = 0.0608]	
Completeness to theta = 24.71°	100.0 %	
Refinement method	Full-matrix least-squares on F2	
Data / restraints / parameters	3398 / 0 / 209	
Goodness-of-fit on F2	1.043	
Final R indices [I>2sigma(I)]	R1 = 0.0524, wR2 = 0.1287	
R indices (all data)	R1 = 0.0709, wR2 = 0.1346	
Extinction coefficient	0.00003(13)	
Largest diff. peak and hole	2.083 and -1.481 e.Å-3	

Table S 15. Atomic coordinates (x 104) and equivalent isotropic displacement parameters (Å2x 103) for Ir2O12C24H32. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ir(1)	3554(1)	4903(1)	3136(1)	39(1)
O(4)	980(9)	5050(3)	2605(8)	49(2)
O(6)	3067(8)	4392(3)	4520(6)	37(2)
O(5)	6119(8)	4711(3)	3614(7)	40(2)
O(3)	4014(8)	5354(3)	1695(6)	42(2)
O(1)	3040(10)	4223(3)	1862(7)	46(2)
O(2)	4673(11)	3566(4)	3208(8)	66(2)
C(7)	4324(15)	4182(4)	5419(10)	40(3)
C(2)	258(13)	5359(5)	1631(10)	44(3)
C(8)	3872(13)	5677(5)	4311(10)	41(3)
C(9)	6901(13)	4453(5)	4624(10)	36(2)
C(4)	2803(16)	5596(5)	846(10)	49(3)
C(12)	3060(20)	3279(6)	1064(13)	81(5)
C(11)	3674(17)	3718(6)	2137(12)	55(3)
C(3)	1088(15)	5618(6)	798(11)	56(3)
C(1)	-1699(13)	5448(6)	1462(11)	60(4)
C(5)	3403(17)	5915(7)	-199(12)	83(5)
C(6)	3738(14)	3745(5)	6223(10)	51(3)
C(10)	8748(13)	4302(6)	4779(11)	58(3)
O(01)	5986(17)	2500	4223(13)	80(4)
Cl(1A)	1326(12)	6889(4)	2154(9)	119(4)
Cl(2A)	-860(20)	7500	3314(16)	198(9)
Cl(5B)	3020(70)	7500	2090(50)	300(30)
Cl(6B)	460(30)	6868(9)	2570(20)	154(9)
Cl(3)	1837(12)	7500	8827(9)	166(3)
Cl(4)	-285(10)	6880(4)	6806(8)	192(3)

C(02)	1010(30)	7500	7160(20)	113(9)

Table S 16. Bond lengths [Å] and angles [°] for Ir2O12C24H32.

Ir(1)-O(3)	1.993(7)
Ir(1)-O(4)	2.003(7)
Ir(1)-O(5)	2.019(6)
Ir(1)-O(6)	2.032(7)
Ir(1)-O(1)	2.069(8)
Ir(1)-C(8)	2.187(12)
O(4)-C(2)	1.272(12)
O(6)-C(7)	1.281(12)
O(5)-C(9)	1.247(11)
O(3)-C(4)	1.264(13)
O(1)-C(11)	1.291(15)
O(2)-C(11)	1.255(14)
C(7)-C(8)#1	1.426(14)
C(7)-C(6)	1.498(14)
C(2)-C(3)	1.394(15)
C(2)-C(1)	1.536(14)
C(8)-C(7)#1	1.426(14)
C(8)-C(9)#1	1.476(14)
C(9)-C(8)#1	1.476(14)
C(9)-C(10)	1.480(13)
C(4)-C(3)	1.356(15)
C(4)-C(5)	1.534(15)
C(12)-C(11)	1.523(16)
C(01)-Cl(6B)	1.67(2)
C(01)-Cl(6B)#2	1.67(2)
C(01)-Cl(1A)	1.726(17)
C(01)-Cl(1A)#2	1.726(17)

C(01)-Cl(2A)	1.88(3)
C(01)-Cl(5B)	1.89(5)
Cl(1A)-Cl(6B)	0.92(2)
Cl(1A)-Cl(5B)	1.99(4)
Cl(2A)-Cl(6B)#2	2.10(3)
Cl(2A)-Cl(6B)	2.10(3)
Cl(5B)-Cl(1A)#2	1.99(4)
Cl(3)-C(02)	1.73(3)
Cl(4)-C(02)	1.767(16)
C(02)-Cl(4)#2	1.767(15)

O(3)-Ir(1)-O(4)	94.9(3)
O(3)-Ir(1)-O(5)	85.5(3)
O(4)-Ir(1)-O(5)	176.6(3)
O(3)-Ir(1)-O(6)	175.8(3)
O(4)-Ir(1)-O(6)	85.4(3)
O(5)-Ir(1)-O(6)	94.0(3)
O(3)-Ir(1)-O(1)	86.6(3)
O(4)-Ir(1)-O(1)	86.9(3)
O(5)-Ir(1)-O(1)	89.7(3)
O(6)-Ir(1)-O(1)	89.2(3)
O(3)-Ir(1)-C(8)	89.5(3)
O(4)-Ir(1)-C(8)	88.1(3)
O(5)-Ir(1)-C(8)	95.3(3)
O(6)-Ir(1)-C(8)	94.8(3)
O(1)-Ir(1)-C(8)	173.3(3)
C(2)-O(4)-Ir(1)	121.7(7)
C(7)-O(6)-Ir(1)	120.6(6)
C(9)-O(5)-Ir(1)	123.7(6)
C(4)-O(3)-Ir(1)	122.0(7)
C(11)-O(1)-Ir(1)	124.4(8)

O(6)-C(7)-C(8)#1	126.7(9)
O(6)-C(7)-C(6)	113.2(9)
C(8)#1-C(7)-C(6)	120.1(9)
O(4)-C(2)-C(3)	126.2(10)
O(4)-C(2)-C(1)	112.8(10)
C(3)-C(2)-C(1)	121.0(10)
C(7)#1-C(8)-C(9)#1	120.5(9)
C(7)#1-C(8)-Ir(1)	105.0(7)
C(9)#1-C(8)-Ir(1)	105.6(7)
O(5)-C(9)-C(8)#1	124.0(9)
O(5)-C(9)-C(10)	117.1(9)
C(8)#1-C(9)-C(10)	118.8(9)
O(3)-C(4)-C(3)	127.3(10)
O(3)-C(4)-C(5)	114.5(10)
C(3)-C(4)-C(5)	118.1(11)
O(2)-C(11)-O(1)	125.4(12)
O(2)-C(11)-C(12)	119.4(12)
O(1)-C(11)-C(12)	115.1(11)
C(4)-C(3)-C(2)	127.9(11)
Cl(6B)-C(01)-Cl(6B)#2	125(2)
Cl(6B)-C(01)-Cl(1A)	31.5(9)
Cl(6B)#2-C(01)-Cl(1A)	128.7(19)
Cl(6B)-C(01)-Cl(1A)#2	128.7(19)
Cl(6B)#2-C(01)-Cl(1A)#2	31.5(9)
Cl(1A)-C(01)-Cl(1A)#2	112.4(17)
Cl(6B)-C(01)-Cl(2A)	72.4(14)
Cl(6B)#2-C(01)-Cl(2A)	72.4(14)
Cl(1A)-C(01)-Cl(2A)	102.2(12)
Cl(1A)#2-C(01)-Cl(2A)	102.2(12)
Cl(6B)-C(01)-Cl(5B)	97.9(17)
Cl(6B)#2-C(01)-Cl(5B)	97.9(17)

Cl(1A)-C(01)-Cl(5B)	66.4(12)
Cl(1A)#2-C(01)-Cl(5B)	66.4(12)
Cl(2A)-C(01)-Cl(5B)	156(2)
Cl(6B)-Cl(1A)-C(01)	70.9(17)
Cl(6B)-Cl(1A)-Cl(5B)	132(2)
C(01)-Cl(1A)-Cl(5B)	60.8(14)
C(01)-Cl(2A)-Cl(6B)#2	49.2(8)
C(01)-Cl(2A)-Cl(6B)	49.2(8)
Cl(6B)#2-Cl(2A)-Cl(6B)	89.7(15)
C(01)-Cl(5B)-Cl(1A)	52.7(13)
C(01)-Cl(5B)-Cl(1A)#2	52.7(13)
Cl(1A)-Cl(5B)-Cl(1A)#2	92(2)
Cl(1A)-Cl(6B)-C(01)	78(2)
Cl(1A)-Cl(6B)-Cl(2A)	132(2)
C(01)-Cl(6B)-Cl(2A)	58.4(13)
Cl(3)-C(02)-Cl(4)	104.7(11)
Cl(3)-C(02)-Cl(4)#2	104.7(11)
Cl(4)-C(02)-Cl(4)#2	111.0(15)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1 #2 x,-y+3/2,z

Table S 17. Anisotropic displacement parameters (Å2x 103) for Ir2O12C24H32. The anisotropic displacement factor exponent takes the form: -2□2[h2 a*2U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Ir(1)	30(1)	45(1)	39(1)	6(1)	9(1)	2(1)
O(4)	31(4)	59(6)	57(5)	-2(4)	9(4)	6(4)
O(6)	33(4)	41(4)	41(4)	5(3)	13(3)	4(3)

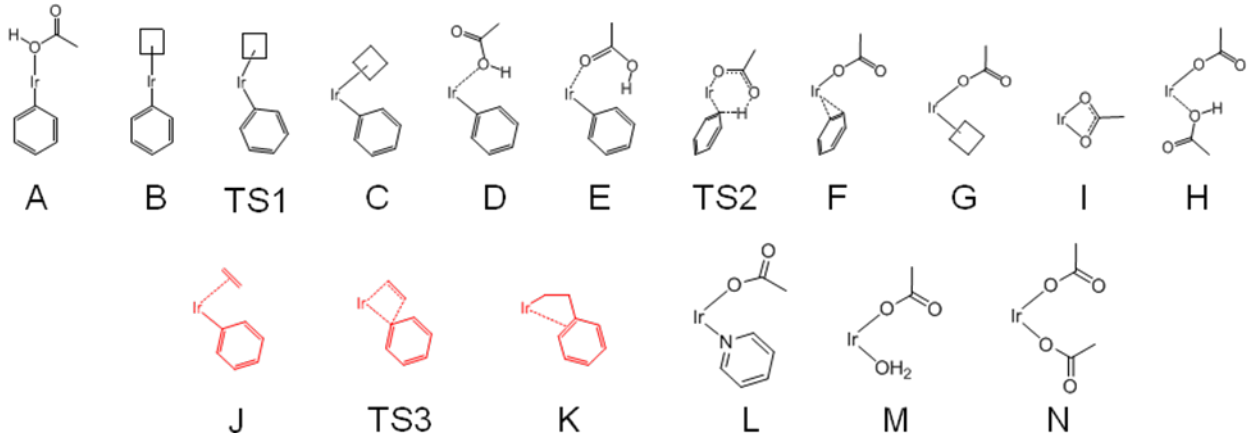
O(5)	29(4)	52(5)	41(4)	6(4)	12(3)	5(4)
O(3)	35(4)	52(5)	37(4)	15(4)	9(3)	16(4)
O(1)	56(5)	48(5)	36(4)	0(4)	14(4)	-2(4)
O(2)	72(6)	54(6)	62(6)	4(5)	3(5)	-4(5)
C(7)	52(7)	36(7)	36(6)	-3(5)	19(5)	-6(6)
C(2)	29(6)	60(8)	38(6)	8(6)	-1(5)	9(6)
C(8)	36(6)	55(8)	34(6)	6(5)	14(5)	0(5)
C(9)	31(6)	37(6)	39(6)	-2(5)	11(5)	0(5)
C(4)	60(8)	60(8)	33(6)	-1(6)	23(6)	-1(7)
C(12)	112(13)	53(9)	78(10)	-10(8)	23(9)	2(9)
C(11)	62(8)	53(9)	57(8)	-8(7)	29(7)	-14(7)
C(3)	52(7)	74(10)	37(7)	16(6)	5(6)	8(7)
C(1)	36(6)	88(11)	47(7)	-9(7)	-4(5)	12(7)
C(5)	64(9)	117(13)	71(9)	42(9)	23(7)	-3(9)
C(6)	46(7)	62(8)	44(7)	12(6)	9(5)	-6(6)
C(10)	39(7)	77(10)	58(8)	14(7)	14(6)	17(6)

Table S 18. Hydrogen coordinates (x 104) and isotropic displacement parameters (Å2x 10 3) for Ir2O12C24H32.

	x	y	z	U(eq)
H(12A)	4013	3037	1034	122
H(12B)	2622	3471	248	122
H(12C)	2142	3053	1233	122
H(3)	380	5833	128	67
H(1A)	-2157	5127	1814	90
H(1B)	-2297	5485	558	90
H(1C)	-1865	5788	1910	90

H(5A)	4315	5703	-410	124
H(5B)	3832	6284	119	124
H(5C)	2437	5956	-961	124
H(6A)	3889	3891	7081	77
H(6B)	4421	3405	6268	77
H(6C)	2529	3658	5836	77
H(10A)	9207	4538	4223	87
H(10B)	8824	3909	4552	87
H(10C)	9410	4361	5664	87
H(02)	1943	7500	6727	136

Density Functional Theory Calculations



A (HOAc)

Gas phase Energy: -1098.62729653212 hartrees

Solvation Energy: -1098.64662739043 hartrees

Zero Point Energy: 170.513 kcal/mol

Coordinates:

Ir1	0.0946972832	0.5844187474	0.2443357233
O2	2.4432357516	0.9070904978	0.4431597319
O3	0.1680764459	-0.5616376860	1.9344666924

C4	0.3268238233	-1.8217235202	1.8645219596
C5	0.5054819474	-2.6197013744	0.7247423067
C6	0.5666401370	-2.1683311185	-0.5951883582
O7	0.4696082854	-0.9731343745	-1.0381682651
H8	0.7303418207	-2.9219527655	-1.3753707003
H9	0.6141854272	-3.6868156835	0.8851977962
H10	0.3278766391	-2.3283924405	2.8371707418
O11	0.0885366778	1.7522660895	-1.4453691395
C12	-0.1515306525	3.0061534405	-1.3677526728
C13	-0.3823783638	3.7823601776	-0.2310237411
C14	-0.3865343230	3.3266718240	1.0961496139
O15	-0.2062747956	2.1452811432	1.5305160356
H16	-0.5580575875	4.0724949047	1.8816847194
H17	-0.5677282328	4.8395159397	-0.3870715827
H18	-0.1613721548	3.5198805670	-2.3367705881
C19	-1.8861077119	0.2910266421	0.0893755017
C20	-2.4753069993	0.0217447627	-1.1575401704
C21	-3.8528581378	-0.1825500524	-1.2687413698
C22	-4.6700768233	-0.1221892324	-0.1391136578
C23	-4.0955964006	0.1445035203	1.1045773396
C24	-2.7182924898	0.3490647268	1.2198426713
H25	-2.2852137848	0.5555749820	2.1940081565
H26	-4.7212111336	0.1945230464	1.9931474388
H27	-5.7418143465	-0.2809012261	-0.2270332669
H28	-4.2874389586	-0.3896665659	-2.2443541288
H29	-1.8511060669	-0.0281603512	-2.0446942004
C30	3.3277640659	0.8871630429	-0.3945230546

C31	3.1386643151	0.7040401378	-1.8818356073
H32	3.5645942598	-0.2590383557	-2.1855328981
H33	2.0806802807	0.7249973493	-2.1346789420
H34	3.6675048338	1.4934577164	-2.4279936995
O35	4.5975251347	1.0284524615	0.0355075773
H36	5.2103646770	0.9985310068	-0.7130568435

B (HOAc)

Gas phase Energy: -869.52774365051 hartrees

Solvation Energy: -869.54615359284 hartrees

Zero Point Energy: 130.711 kcal/mol

Coordinates:

Ir1	0.0700006699	-0.6177493485	-0.0000192679
O2	1.5656269736	-0.5228717847	1.3863121574
C3	1.3128091234	-0.5348548579	2.6380939154
C4	0.0729441886	-0.6519406755	3.2746916964
C5	-1.1612550993	-0.8156507479	2.6374755527
O6	-1.4094535049	-0.8600852400	1.3854551553
H7	-2.0463599643	-0.9374660556	3.2723865405
H8	0.0714420490	-0.6410875980	4.3589573977
H9	2.2022783994	-0.4549928288	3.2735628345
O10	-1.4100598776	-0.8599478067	-1.3848596758
C11	-1.1623628188	-0.8157418486	-2.6369721822
C12	0.0715872846	-0.6521086375	-3.2747100879
C13	1.3117219086	-0.5350398133	-2.6386320492
O14	1.5650475017	-0.5227006940	-1.3869512934
H15	2.2009550095	-0.4555010385	-3.2744667117

H16	0.0696392130	-0.6414098799	-4.3589785500
H17	-2.0477198693	-0.9377147379	-3.2715061941
C18	-0.1544135053	1.3733794837	0.0000538397
C19	-1.4378646029	1.9360248241	-0.0016811631
C20	-1.5873781973	3.3255686698	-0.0017183930
C21	-0.4687618729	4.1595467167	0.0000584246
C22	0.8075505364	3.5957105507	0.0018429250
C23	0.9714556145	2.2077830708	0.0018449647
H24	1.9666976929	1.7765188098	0.0032326013
H25	1.6866682728	4.2357311667	0.0032294650
H26	-0.5905520704	5.2393502105	0.0000268149
H27	-2.5869959201	3.7536303480	-0.0031503434
H28	-2.3119866496	1.2938413281	-0.0030488099

C (HOAc)

Gas phase Energy: -869.49314648211 hartrees

Solvation Energy: -869.50611536686 hartrees

Zero Point Energy: 130.357 kcal/mol

Coordinates:

Ir1	-0.1963584177	0.0870646895	-0.2128938346
O2	1.2562363879	0.2826972169	-1.6408194052
O3	1.2273668153	0.0483112304	1.1528518139
C4	0.9304339585	-0.0920403826	2.3981962179
C5	-0.3116818202	-0.2345996808	3.0005931613
C6	-1.5469457435	-0.2669078612	2.3315489836
O7	-1.7516634413	-0.1479101773	1.0840992403
H8	-2.4500561458	-0.4123454608	2.9341194951

H9	-0.3261695890	-0.3462421898	4.0787291174
H10	1.8218201486	-0.1008302950	3.0321110747
C11	-0.4487562423	2.0829821869	-0.2353405417
C12	-1.7476774443	2.6228050180	-0.1592360139
C13	-1.9678066567	3.9964273205	-0.3013497938
C14	-0.8920103847	4.8628125440	-0.4883092571
C15	0.4068233276	4.3465462469	-0.5386449818
C16	0.6252470079	2.9756795303	-0.4151525281
H17	1.6377182713	2.5864094101	-0.4706315718
H18	1.2515861647	5.0171867899	-0.6782859884
H19	-1.0601591841	5.9320246953	-0.5864450875
H20	-2.9813517092	4.3873707761	-0.2519307310
H21	-2.5964085235	1.9663626617	0.0169585674
O22	-0.0463060977	-2.1116041078	-0.2672165726
C23	0.8518733486	-2.6751838126	-0.9533502459
C24	1.9237772432	-0.7174645686	-2.0881636288
C25	1.8030720879	-2.0751669772	-1.8026983187
H26	0.8866602620	-3.7738068552	-0.8852051948
H27	2.6948816905	-0.4299471412	-2.8126789637
H28	2.4950169016	-2.7393387632	-2.3097346028

D (HOAc)

Gas phase Energy: -1098.61810593984 hartrees

Solvation Energy: -1098.62874904375 hartrees

Zero Point Energy: 170.591 kcal/mol

Coordinates:

Ir1	0.0873231374	-0.0495998346	0.2670474928

O2	0.6589642073	-0.3182910867	2.2227253977
O3	2.0394236399	0.0024199050	-0.1767100498
C4	2.4244921285	0.1667965119	-1.3856845650
C5	1.6557172434	0.3355325669	-2.5394299671
C6	0.2584734161	0.3749471174	-2.6007598588
O7	-0.5743651829	0.2472405360	-1.6429775114
H8	-0.2027052824	0.5384789186	-3.5811542604
H9	2.1936961268	0.4621061108	-3.4722281639
H10	3.5138957048	0.1770929716	-1.4935957071
C11	0.0072162448	-2.0647002622	0.0451268554
C12	-1.0009930142	-2.6828289821	-0.7204408597
C13	-1.0779849425	-4.0766937433	-0.8337412402
C14	-0.1391540739	-4.8843820532	-0.1966097843
C15	0.8773118364	-4.2875730191	0.5551941731
C16	0.9470349245	-2.9001569167	0.6772332736
H17	1.7362265145	-2.4544390250	1.2751984770
H18	1.6186648175	-4.9086368039	1.0531028067
H19	-0.1926808271	-5.9660388026	-0.2867524664
H20	-1.8684748682	-4.5244545762	-1.4315532277
H21	-1.7210115295	-2.0753568177	-1.2658936486
O22	0.2017235104	2.1491667145	0.4526402285
C23	0.6401253106	2.6705900011	1.5197931260
C24	0.9989642991	0.6587345214	2.9731214062
C25	1.0206824929	2.0308243473	2.7121432502
H26	0.7245497446	3.7688714833	1.5122760715
H27	1.3155621528	0.3449100778	3.9756728470
H28	1.3655880438	2.6685685039	3.5192435541

O29	-2.0239507058	-0.1975049289	0.8247680353
H30	-2.2182181954	-1.1576620339	0.7798580259
C31	-3.1070608078	0.4715975565	0.2237477966
O32	-4.0472009327	-0.1722271897	-0.1516442149
C33	-2.9302450629	1.9567904430	0.1974188696
H34	-2.0172480584	2.2249767865	-0.3388056370
H35	-3.8062859892	2.4012473564	-0.2735457850
H36	-2.8220348181	2.3300290501	1.2205129392

E (HOAc)

Gas phase Energy: -1098.63868153017 hartrees

Solvation Energy: -1098.64959916325 hartrees

Zero Point Energy: 170.835 kcal/mol

Coordinates:

Ir1	0.2578644090	-1.2689813445	-0.3085648701
C2	0.4999388716	-3.1954565769	-0.8922144739
C3	0.8236486456	-5.8835887299	-1.7252617729
C4	1.2951404871	-4.0942915464	-0.1591309860
C5	-0.1246069717	-3.6773579899	-2.0566053590
C6	0.0346128628	-5.0030048307	-2.4675950909
C7	1.4539829881	-5.4212830649	-0.5689579460
H8	1.8039093186	-3.7492791137	0.7375367374
H9	-0.7402407327	-3.0057366737	-2.6482755453
H10	-0.4589367153	-5.3474331797	-3.3739059847
H11	2.0771520515	-6.0939460421	0.0165695238
H12	0.9482402019	-6.9145732174	-2.0457384371
H13	-2.0143714089	-2.4675680545	0.4683845632

O14	-2.0756548112	-2.8611975269	1.3851676172
C15	-1.0194436936	-2.5558501702	2.0975547750
C16	-1.0511896608	-3.0555541980	3.5109732580
O17	-0.0471201116	-1.9008258945	1.6791023816
H18	-0.1638034032	-2.7199440644	4.0454716101
H19	-1.9559073755	-2.6949092720	4.0089624820
H20	-1.0934692395	-4.1490798262	3.5030289407
C21	3.0902077446	-0.7408339934	-0.5894094552
O22	2.2084413691	-1.1378808000	0.2398953463
H23	4.1043679576	-0.7001802450	-0.1761978549
C24	-2.5252758698	-0.3483116985	-0.8519098256
O25	-1.7653704931	-1.3993782888	-0.7889385779
H26	-3.5410141197	-0.5726080601	-1.1954353833
C27	-1.0268100024	1.4879411685	-0.0140632495
C28	-2.2401693631	0.9674786273	-0.5420743393
H29	-1.0307848570	2.5676184448	0.2092047455
H30	-3.0456695830	1.6799036696	-0.6879390943
O31	0.0369691232	0.8757645311	0.2419258633
C32	1.7087402832	-0.3160956251	-2.6173894033
C33	2.9201315635	-0.3558292321	-1.9251477725
H34	1.7295620424	0.0213122983	-3.6594088963
H35	3.8080622874	-0.0503677437	-2.4672606374
O36	0.5382159176	-0.6171038879	-2.2000459750

F (HOAc)

Gas phase Energy: -1098.61172674620 hartrees

Solvation Energy: -1098.62656218465 hartrees

Zero Point Energy: 170.647 kcal/mol

Coordinates:

Ir1	0.5357197718	-0.9458607422	-0.0540413667
O2	1.8971563345	-1.2873776202	1.4906151118
C3	1.5801389654	-2.0543757640	2.4590789914
C4	0.3530451045	-2.6648096158	2.7323238867
C5	-0.8185606210	-2.5461814191	1.9718421709
O6	-1.0149352208	-1.8996131127	0.8949075097
H7	-1.7071635197	-3.0728831256	2.3411064562
H8	0.2993621000	-3.2838044433	3.6211965852
H9	2.3978310750	-2.2409471201	3.1669747227
O10	2.0844265936	0.0119237014	-0.9851276010
C11	-1.7770321344	1.3188145159	0.2823375245
C12	-0.3621716268	1.3291732055	0.1335611634
H13	-2.3968265313	1.4648976978	-0.5959964916
H14	0.0676200244	1.6130274267	-0.8216552714
C15	-2.3453984904	1.1457962524	1.5245382868
C16	0.4492089032	1.1548777687	1.2749389296
C17	-1.5270040831	0.9820248743	2.6675041967
C18	-0.1535321721	0.9871456842	2.5508429691
H19	-1.9887877502	0.8605866283	3.6438081127
H20	0.4762374678	0.8812416335	3.4286194247
H21	-3.4260652574	1.1455672845	1.6355715451
H22	1.5191126810	1.3133439261	1.2028334983
O23	1.0508310549	-2.7960445085	-0.6981141876
C24	2.0448920428	-2.9505345129	-1.4914536086
C25	2.9028346136	-0.6253836839	-1.7162441068

C26	2.9237246861	-1.9990508359	-2.0027773733
H27	2.2006722788	-3.9945704050	-1.7841561190
H28	3.6836411375	-0.0016040083	-2.1652091214
H29	3.7063087856	-2.3550337221	-2.6628773213
C31	-0.7181472755	-0.1871148659	-2.6979600357
O32	-0.7486433999	-0.9789694992	-1.6510846873
O33	-0.0240629919	0.8153349968	-2.8470850614
C34	-1.6878725198	-0.6608685192	-3.7778752529
H35	-1.7724809854	0.0973517318	-4.5573973352
H36	-1.3193511274	-1.5937791735	-4.2169031192
H37	-2.6693306250	-0.8737333509	-3.3455774675

G (HOAc)

Gas phase Energy: -866.33468783032 hartrees

Solvation Energy: -866.36257656368 hartrees

Zero Point Energy: 106.201 kcal/mol

Coordinates:

Ir1	0.4203318637	-1.1063929381	-0.0361842165
O2	1.9349206964	-1.1603204035	1.3881221111
C3	1.7611358481	-1.7731542728	2.4921937587
C4	0.6087467218	-2.4112971196	2.9657838616
C5	-0.6272398921	-2.4771753740	2.3133912184
O6	-0.9575364155	-2.0156720051	1.1702188897
H7	-1.4467370109	-2.9795263749	2.8401271875
H8	0.6720511114	-2.8778046115	3.9424826011
H9	2.6406901214	-1.7771893258	3.1475504005
O10	1.7197648953	-0.0664902921	-1.2022010366

O23	1.0961125044	-2.9022461466	-0.5070541042
C24	2.1064931102	-3.0202042183	-1.2987938731
C25	2.6298158417	-0.6644524207	-1.8555008310
C26	2.8702745704	-2.0453270529	-1.9196232440
H27	2.3617589632	-4.0700760756	-1.4687023550
H28	3.2874637825	-0.0030257840	-2.4290218710
H29	3.6884055356	-2.3822203793	-2.5450867157
C31	-1.0790436037	-1.0050180177	-2.5610555532
O32	-1.1181173730	-0.7541372114	-1.2576301330
O33	-0.1723681660	-1.5980883338	-3.1234721260
C34	-2.3223298009	-0.5094805484	-3.2780295748
H35	-2.1865779737	-0.6026177251	-4.3560843634
H36	-3.1847243057	-1.1083988819	-2.9675599638
H37	-2.5333682122	0.5294926315	-3.0105479355

H (HOAc)

Gas phase Energy: -866.37817997799 hartrees

Solvation Energy: -866.39116123403 hartrees

Zero Point Energy: 106.763 kcal/mol

Coordinates:

Ir1	-0.2448582480	0.0129534285	-0.2315559389
O2	1.1814382611	0.3349671627	-1.6581543321
O3	1.2643769379	0.0826913128	1.1392167638
C4	1.0195835354	-0.0625539146	2.3838267995
C5	-0.2087849082	-0.2623309703	3.0182752244
C6	-1.4567792133	-0.3377364183	2.3884074691
O7	-1.7296966580	-0.2452300114	1.1476531759

H8	-2.3343662219	-0.4916295303	3.0271191190
H9	-0.1947808894	-0.3630998749	4.0976685629
H10	1.9131203665	-0.0113607067	3.0163558911
O22	0.0529313889	-2.0030582031	-0.1308659106
C23	0.9505295797	-2.5643107318	-0.8446233740
C24	1.8896102961	-0.6273697624	-2.0995842503
C25	1.8295372759	-1.9849846850	-1.7629151146
H26	1.0148934852	-3.6484414927	-0.6971951226
H27	2.6345319369	-0.3265050045	-2.8454276978
H28	2.5242756548	-2.6483350502	-2.2656770445
C18	-1.7303211829	1.6075674514	-1.4414875327
O19	-0.8984297615	2.0023165621	-0.5523413788
O20	-1.7557227795	0.3503642288	-1.6745082770
C21	-2.6221506470	2.5667412649	-2.1652695155
H22	-3.2516204681	2.0325226649	-2.8773544657
H23	-3.2457875269	3.1004493669	-1.4422610959
H24	-2.0110699771	3.3081764033	-2.6880469817

I (HOAc)

Gas phase Energy: -1095.48783217819 hartrees

Solvation Energy: -1095.50293319691 hartrees

Zero Point Energy: 146.080 kcal/mol

Coordinates:

Ir1	0.1130048873	0.0968045297	0.0885416610
O2	0.6127802884	-0.7869177820	1.8624218298
O3	2.1119296510	0.3380838926	-0.2504855006
C4	2.5365117074	0.8498279072	-1.3388365740

C5	1.8012495426	1.3125984338	-2.4349583054
C6	0.4082319185	1.3059897137	-2.5493462116
O7	-0.4579356745	0.8862744129	-1.7114788878
H8	-0.0254208488	1.7081152302	-3.4720279790
H9	2.3626154048	1.7146500947	-3.2707054914
H10	3.6284967699	0.9242369311	-1.3956519190
O11	0.0709825148	1.9824524672	0.8417725433
C12	0.3548462728	2.2061862916	2.0686469074
C13	0.7824684556	-0.0940970515	2.9165773413
C14	0.6810487294	1.2942911726	3.0726883033
H15	0.3235558242	3.2677847148	2.3375867310
H16	1.0464944502	-0.6841710250	3.8016133589
H17	0.8788440353	1.6965401552	4.0597183890
O18	-1.8751035610	-0.3310875328	0.5387624670
H19	-1.8703320046	-1.7095879301	0.2522606895
C20	-3.0212569035	0.3103916203	0.2222765761
O21	-4.0400546626	-0.3277331162	0.0516477868
C22	-2.9666098656	1.8214264800	0.1601444688
H23	-2.2497667187	2.1496031166	-0.5951488510
H24	-3.9624680423	2.1964577306	-0.0771128522
H25	-2.6371590628	2.2268973064	1.1206380296
O26	0.3012763380	-1.7940373846	-0.7899892442
C27	-0.5018887424	-2.7569130735	-0.6624676013
O28	-1.6425920055	-2.7013167165	-0.0708879104
C29	-0.1187420500	-4.0939502187	-1.2333263992
H30	0.8150500448	-4.0209963173	-1.7892651587
H31	-0.0063771549	-4.8091496417	-0.4123136914

H32	-0.9228620942	-4.4592629899	-1.8775579379

J (HOAc)

Gas phase Energy: -948.14279053823 hartrees

Solvation Energy: -948.14472425646 hartrees

Zero Point Energy: 165.423 kcal/mol

Coordinates:

Ir1	-0.3101382620	0.0630332550	-0.1623546766
O2	-1.9844536357	-0.1053004030	-1.3529912885
O3	0.7864692165	0.2582846355	-1.9162924847
C4	2.0554188374	0.3645113438	-1.8774314529
C5	2.9028061214	0.3723411466	-0.7644713168
C6	2.5095308236	0.2675627714	0.5724767742
O7	1.3339854148	0.1645210419	1.0585238867
H8	3.3019097147	0.2761507846	1.3299616976
H9	3.9659483633	0.4631680000	-0.9570624129
H10	2.5272609243	0.4558892488	-2.8635897568
C11	-0.4451820032	2.1301680227	-0.2456779759
C12	-1.1063926370	2.7322202369	-1.3262333076
C13	-1.1133429038	4.1216012041	-1.4808885680
C14	-0.4614588123	4.9414372574	-0.5591561038
C15	0.1969788215	4.3549251175	0.5221158618
C16	0.2019152460	2.9658581187	0.6774369880
H17	0.7243825252	2.5335875744	1.5261325629
H18	0.7119950939	4.9775859869	1.2502348602
H19	-0.4659355555	6.0212001689	-0.6817492019
H20	-1.6311234019	4.5621613737	-2.3299817754

H21	-1.6170991889	2.1127149948	-2.0553876328
O22	0.2257577818	-2.0570474752	-0.4640071465
C23	-0.4436109377	-2.7619459850	-1.2712201273
C24	-2.2598268121	-1.1851193086	-1.9816137795
C25	-1.6043161890	-2.4163523584	-1.9886053539
H26	-0.0686596847	-3.7860337921	-1.4232680284
H27	-3.1597849613	-1.1046454307	-2.6037159108
H28	-2.0332898520	-3.1864215320	-2.6207651027
C29	-1.6237076916	0.5053249854	1.5621955938
C30	-1.3874629872	-0.8677951436	1.5023623906
H31	-1.0728212789	1.1278729296	2.2576701515
H32	-0.6338430743	-1.3261087186	2.1351776688
H33	-2.1253426647	-1.5399425835	1.0741619586
H34	-2.5425209743	0.9286670080	1.1707768631

K (HOAc)

Gas phase Energy: -948.13867877898 hartrees

Solvation Energy: -948.14588847230 hartrees

Zero Point Energy: 166.004 kcal/mol

Coordinates:

Ir1	-0.4747231409	0.0914632909	-0.3423317569
O2	-1.2323222728	0.2375391648	-2.2541333524
O3	1.3239358176	0.0406396806	-1.2731343601
C4	2.4081947070	-0.1098116763	-0.6127708617
C5	2.5850322939	-0.2343324591	0.7652350868
C6	1.5616140535	-0.2120772888	1.7221327730
O7	0.3107816037	-0.0689057571	1.5399559130

H8	1.8533027767	-0.3277413153	2.7731193794
H9	3.5998126835	-0.3614206126	1.1255400845
H10	3.3022144507	-0.1412079034	-1.2458532219
O11	-0.3970389409	-2.1310047711	-0.4303306927
C12	-0.6887148949	-2.7118148628	-1.5101093043
C13	-1.3660754575	-0.7977031733	-2.9977023091
C14	-1.1449104167	-2.1460279736	-2.7207678837
H15	-0.5781029009	-3.8092599556	-1.5092673182
H16	-1.7198347111	-0.5602684201	-4.0092373974
H17	-1.3361333496	-2.8381245842	-3.5346240376
C18	-0.5175582951	2.1728960701	-0.2506011128
H19	0.1949589637	2.5201799400	0.5070932369
H20	-0.2501506212	2.6018836154	-1.2211740621
C21	-1.9647588552	2.5035803988	0.1643813714
H22	-2.0593065212	3.4165357738	0.7653409629
H23	-2.6018557685	2.6185210928	-0.7195680605
C24	-3.0316101316	-1.0870832225	2.3671801931
C25	-3.1300739068	-1.0678116898	0.9905487183
C26	-2.8128923066	0.1088651967	0.2605313904
C27	-2.4033328208	1.2814272544	0.9511713436
C28	-2.3318852463	1.2394962670	2.3592494569
C29	-2.6445233480	0.0815538539	3.0507018081
H30	-3.2621594946	-1.9910455567	2.9227472893
H31	-3.4592334083	-1.9495954721	0.4493595533
H32	-3.1107879665	0.1817108516	-0.7805498498
H33	-2.0195121191	2.1295138148	2.8981085858
H34	-2.5854069120	0.0726390793	4.1360619991

L (HOAc)

Gas phase Energy: -1114.732831 hartrees

Solvation Energy: -1114.475476 hartrees

Zero Point Energy: 163.839 kcal/mol

Coordinates:

Ir1	0.0196113546	-0.0162800024	0.0670120505
O2	-0.0435364411	0.0814731750	2.1431592653
O3	2.0540357018	0.0040066556	0.2488324685
O4	-0.1502914038	-2.0460662198	0.3154285525
O5	-2.0269192892	-0.0156628510	-0.1491084306
C6	-1.1559793890	0.0137341677	2.7598074890
H7	-1.0664783472	0.0207552649	3.8538114285
C8	-2.7898863152	-0.0709727866	0.8672472423
H9	-3.8577594665	-0.1279489850	0.6219199286
C10	2.6875611853	-1.0587589277	0.5732865963
H11	3.7677133826	-0.9081686408	0.6824618238
C12	0.8664550220	-2.7480302030	0.6209576133
H13	0.6452626451	-3.8129343068	0.7613616216
C14	-2.4502609143	-0.0509801765	2.2284325965
H15	-3.2692200110	-0.1053871350	2.9375025242
C16	2.1930678351	-2.3413940941	0.7993949771
H17	2.9125738490	-3.1074784557	1.0655425799
O18	0.0601917174	-0.0113523661	-1.9793168142
C19	0.6936953432	-0.9281757956	-2.6837663140
C20	0.4377684644	-0.7624157732	-4.1788952135
H21	0.4970244715	0.2884883667	-4.4746288871

H22	1.1571745797	-1.3573698198	-4.7435926965
H23	-0.5744140028	-1.1104212553	-4.4114181825
O24	1.3963852849	-1.8270380922	-2.2437721731
N25	0.1285215629	2.0312928107	-0.1366359718
C26	-0.6720861080	2.8626851167	0.5609464761
C27	-0.5898152513	4.2428292465	0.4347712496
C28	0.3503537823	4.7896586736	-0.4379243300
C29	1.1743386584	3.9265310167	-1.1565429252
C30	1.0366158134	2.5544836193	-0.9853390809
H31	-1.3856105454	2.3936406839	1.2274745079
H32	-1.2561646909	4.8711639648	1.0157552248
H33	0.4372084431	5.8655110001	-0.5551220308
H34	1.9203542539	4.3022651495	-1.8483700250
H35	1.6406673822	1.8364005709	-1.5225121961

M (HOAc)

Gas phase Energy: -942.8433504 hartrees

Solvation Energy: -942.833763027 hartrees

Zero Point Energy: 122.927 kcal/mol

Coordinates:

Ir1	0.0310563986	0.0864420823	-0.0046586974
O2	-1.9142284970	-0.1162173549	0.6624971653
O3	0.2223736237	-1.9162588874	0.3090317343
O4	-0.7698824815	-0.0856264594	-1.8383906634
O5	-0.0939219114	2.1264236757	-0.2303132516
C6	-2.7096528821	0.8775155972	0.6593103097
H7	-3.7295491198	0.6370072960	0.9839865537

C8	-1.2105435915	2.7299787440	-0.0842902360
H9	-1.1643424562	3.8055675082	-0.2927832410
C10	-0.2260220351	-2.7523960462	-0.5427776178
H11	-0.0963942194	-3.7995320059	-0.2473434445
C12	-1.0326516738	-1.2362723736	-2.3315841757
H13	-1.4745248501	-1.1825000613	-3.3317945428
C14	-2.4452178697	2.2100077808	0.3148847323
H15	-3.2737167961	2.9067870496	0.3775503717
C16	-0.8411558021	-2.4974985499	-1.7712546935
H17	-1.1447770803	-3.3535679429	-2.3626940383
O18	2.0260379165	0.3033123523	-0.4398259937
C19	2.6294708995	-0.3492985671	-1.4251872280
C20	4.1207324106	-0.0468385927	-1.4799943515
H21	4.5948321965	-0.2761817086	-0.5204937740
H22	4.5852499339	-0.6364094479	-2.2710059798
H23	4.2767686851	1.0187614779	-1.6758314604
O24	2.0772865235	-1.0926973933	-2.2175821242
O25	1.0383533376	0.3964014343	1.8942341401
H26	0.8900252988	1.3182763366	2.1566113270
H27	1.9269116755	0.3837365217	1.4686597813

N (HOAc)

Gas phase Energy: -1094.993769 hartrees

Solvation Energy: -1094.834898 hartrees

Zero Point Energy: 137.682 kcal/mol

Coordinates:

Ir1	0.0757682736	-0.0251305065	0.1366583128

O2	0.2632366948	-0.5606383806	2.1316401276
O3	2.1148574076	-0.2447183246	-0.0244651020
O4	-0.3452088944	-2.0166769514	-0.2982032421
O5	-1.9582783116	0.1823143366	0.2374891434
C6	-0.7683932982	-0.7314768581	2.8565838944
H7	-0.5462739675	-1.0443479210	3.8878375017
C8	-2.5974298677	-0.1204997845	1.2882717518
H9	-3.6863081857	0.0013116836	1.1970792056
C10	2.6186234588	-1.3683211568	-0.3278901564
H11	3.7170098969	-1.3668948161	-0.3898830197
C12	0.5984004582	-2.8258946967	-0.5537541578
H13	0.2701845951	-3.8526225387	-0.7769698723
C14	-2.1146444025	-0.5854864729	2.5192922926
H15	-2.8465249788	-0.7785091243	3.2974167068
C16	1.9793014571	-2.5905271920	-0.5837148921
H17	2.6165793686	-3.4350773020	-0.8277631368
O18	0.0572015718	0.3260386856	-1.8840405045
C19	-0.5512748950	1.3301437122	-2.4626461623
C20	-0.3184565570	1.3001060424	-3.9821605414
H21	-0.5804226777	0.3187998683	-4.3908865167
H22	-0.9163561682	2.0770339931	-4.4639641543
H23	0.7420501800	1.4701696445	-4.1989258903
O24	-1.2257531906	2.2154608362	-1.9525661866
O25	0.5677001444	1.9267412368	0.4731676347
C26	-0.1180727242	2.7229097308	1.2451461443
C27	0.3142415017	4.1793690422	1.0553625136
H28	1.4047262372	4.2640227817	1.0256124809

H29	-0.0716857785	4.5265649777	0.0909584518
H30	-0.0930722846	4.8006863954	1.8567031417
O31	-1.0127048032	2.4253218641	2.0321523365

TS1 (HOAc)

Gas phase Energy: -866.32069123148 hartrees

Solvation Energy: -869.50174871241 hartrees

Zero Point Energy: 105.581 kcal/mol

Coordinates:

Ir1	-0.1148565514	0.0298585447	0.0173092198
O2	-0.1799709914	-0.0211279875	2.0638000339
O3	1.8531712872	-0.2044121988	0.1220490501
C4	2.5566250758	-0.3011368511	-0.9481270981
C5	2.1583573189	-0.2680596910	-2.2791156527
C6	0.8451665225	-0.0783374220	-2.7224209423
O7	-0.2015917600	0.0816268037	-2.0138564456
H8	0.6695899164	-0.0340263425	-3.8025365450
H9	2.9315820171	-0.3749299963	-3.0304522561
H10	3.6204478444	-0.4211677210	-0.7265198286
O11	-0.7368518229	2.0828610038	-0.0091538270
C12	-0.9305120236	2.7361057249	1.0725064701
C13	-0.4434628097	0.9944412407	2.7854691128
C14	-0.7817008473	2.2956936869	2.3899969418
H15	-1.2634841033	3.7725775771	0.9294796047
H16	-0.3879797153	0.7944369145	3.8619304383
H17	-0.9764477211	3.0128809759	3.1795824677
C18	0.3259516981	-2.9727731461	-0.3011218408

O19	-0.4317044971	-1.9575092365	0.0834092884
O20	1.4469921034	-2.9084993205	-0.7777242633
C21	-0.3956494003	-4.2954305014	-0.0660453514
H22	0.2364115711	-5.1159602564	-0.4078086764
H23	-0.6179405111	-4.4159728100	0.9983211637
H24	-1.3481973520	-4.3087765125	-0.6038254853

TS2 (HOAc)

Gas phase Energy: -1098.60886828523 hartrees

Solvation Energy: -1098.62050353405 hartrees

Zero Point Energy: 167.510 kcal/mol

Coordinates:

Ir1	0.0697647218	-1.3363898764	-0.1675870619
C2	0.2229288551	-3.4797894422	-0.7013835559
C3	1.1060651068	-5.5406420487	-2.4111092874
C4	1.4371969161	-4.1624416477	-0.4577503591
C5	-0.5487428775	-3.8847775446	-1.8142123020
C6	-0.1119447380	-4.9004601178	-2.6597384374
C7	1.8777501463	-5.1755227286	-1.3039470623
H8	2.0216331558	-3.8953213144	0.4182967077
H9	-1.4927624817	-3.3841075034	-2.0040601716
H10	-0.7157445672	-5.1951999327	-3.5132314367
H11	2.8152613973	-5.6865986144	-1.1022485426
H12	1.4481267215	-6.3324707917	-3.0725552701
H13	-0.4198933724	-3.3632986118	0.3771585631
O14	-1.0232042787	-3.6083819973	1.6706396226
C15	-0.9478183788	-2.5285992541	2.3045709561

C16	-1.4002393504	-2.4779494410	3.7474688615
O17	-0.5068568895	-1.4270213923	1.8124456183
H18	-1.1602161559	-1.5155724761	4.1997633382
H19	-2.4812521995	-2.6438374177	3.7874929407
H20	-0.9235955926	-3.2886833523	4.3047129795
C21	2.9650765661	-1.0267441748	-0.3153502454
O22	2.0126310023	-1.3023285121	0.4856819497
H23	3.9505180675	-0.9849696838	0.1641293624
C24	-2.5768503175	-0.2805030680	-0.8072561327
O25	-1.8992309892	-1.3601617484	-0.7412627168
H26	-3.6138911831	-0.4289194432	-1.1309669440
C27	-0.9021777346	1.4300775777	-0.1051711322
C28	-2.1762089725	1.0280227779	-0.5269592413
H29	-0.7506390280	2.5028587958	0.0703022082
H30	-2.9218538268	1.8058499482	-0.6484083156
O31	0.1297221330	0.7184210989	0.1088594915
C32	1.7598185665	-0.7862697226	-2.4844778643
C33	2.9129303608	-0.7863368907	-1.6924045899
H34	1.8864886656	-0.5823929422	-3.5547019338
H35	3.8526200471	-0.5764582419	-2.1912780635
O36	0.5510344503	-0.9899070143	-2.1367115566

TS3 (HOAc)

Gas Phase Energy: -948.10254973374 hartrees

Solvation Energy: -948.10959259066 hartrees

Zero Point Energy: 164.537 kcal/mol

Coordinates:

Ir1	-.0179673153	.0603133507	.0114309977
O2	-.0758930265	.0346857438	2.0697719582
O3	2.1444722267	-.2091755006	.1243285837
C4	2.8372676698	-.1811490654	-.9300059438
C5	2.4091937648	.0036332836	-2.2612659744
C6	1.0974517512	.1559963757	-2.7035070352
O7	-.0007724021	.1492244331	-2.0437844606
H8	.9529715708	.2855598521	-3.7834591780
H9	3.1811912316	.0208616011	-3.0233886802
H10	3.9205952719	-.3173245912	-.7870147447
C11	-.3422212543	-2.1170318833	-.0238085169
C12	.0618791115	-2.8119843248	1.1372313724
C13	.6185964193	-4.0866269832	1.0549837956
C14	.7712476326	-4.7098955126	-.1872002237
C15	.3581540173	-4.0473112516	-1.3490379850
C16	-.1990255679	-2.7748253581	-1.2668876894
H17	-.5354543549	-2.2725169613	-2.1682595285
H18	.4656730408	-4.5274162307	-2.3180219589
H19	1.2000484338	-5.7061660271	-.2498770701
H20	.9361313829	-4.5937878725	1.9621181057
H21	-.0465763759	-2.3286005503	2.1021502665
O22	.4840109963	2.0695404126	-.0867250349
C23	.6296752114	2.7640000170	.9675538104
C24	.1785258270	1.0828278602	2.7528268026
C25	.5034913376	2.3653642147	2.3060036468
H26	.8869704908	3.8148296697	.7823948326
H27	.1229284364	.9301502945	3.8374025058

H28	.6759149180	3.1213441533	3.0641340064
C29	-2.0219520904	-1.2516270304	.1489970272
C30	-2.0827809139	.2013052222	-.0335885828
H31	-2.4804932520	-1.8619762692	-.6225842431
H32	-2.4461800454	.5504636942	-.9997433307
H33	-2.4773919748	.7702980183	.8088481216
H34	-2.2407690250	-1.6067214348	1.1516316428

A (HTFA)

Gas phase Energy: -1396.37518848232 hartrees

Solvation Energy: -1396.33615546378 hartrees

Zero Point Energy: 156.102 kcal/mol

Coordinates:

Ir1	0.0237955319	0.6387912979	0.1924430103
O2	2.4030880389	1.1331062803	0.2989585536
O3	0.1920923690	-0.5508309192	1.8487926814
C4	0.3596947752	-1.8088015830	1.7400189609
C5	0.4957832685	-2.5748794732	0.5753078039
C6	0.4900072364	-2.0870596643	-0.7349015402
O7	0.3547867592	-0.8839774000	-1.1390926176
H8	0.6330279628	-2.8155266023	-1.5420768247
H9	0.6284956265	-3.6437491579	0.7022208414
H10	0.4110818897	-2.3382145735	2.6991378322
O11	-0.0678598855	1.8545470777	-1.4552530021
C12	-0.3023518340	3.1032985883	-1.3317023088
C13	-0.4797552057	3.8500129077	-0.1631050672

C14	-0.4265459441	3.3551206350	1.1463703941
O15	-0.2275399624	2.1592553830	1.5361241281
H16	-0.5632834166	4.0751935589	1.9621705851
H17	-0.6673120359	4.9117405858	-0.2806566830
H18	-0.3555043610	3.6437020854	-2.2848070858
C19	-1.9504143150	0.3139496719	0.1094190634
C20	-2.5783668845	0.0712644143	-1.1230758222
C21	-3.9545235125	-0.1592778760	-1.1863440975
C22	-4.7269765805	-0.1517165441	-0.0240112663
C23	-4.1105813959	0.0899766475	1.2045113453
C24	-2.7343955118	0.3217394683	1.2740929079
H25	-2.2660389025	0.5082649360	2.2354903400
H26	-4.7018356239	0.0987902258	2.1174171026
H27	-5.7975390933	-0.3321291713	-0.0754179768
H28	-4.4223690801	-0.3459391349	-2.1504692210
H29	-1.9870223520	0.0627427160	-2.0333311965
C30	3.3964455065	1.0962122367	-0.3862837350
C31	3.4485165685	0.3322312934	-1.7366322888
F32	3.3380528688	-0.9813274230	-1.5220069529
F33	2.4917435199	0.7401015280	-2.5569251157
F34	4.6544743134	0.5547719835	-2.3368788810
O35	4.5315022721	1.6881328942	-0.0258412858
H36	5.2059241277	1.5575742600	-0.7130611203

B (HTFA)

Gas phase Energy: -869.55690970873 hartrees

Solvation Energy: -869.54753503974 hartrees

Zero Point Energy: 130.711 kcal/mol

Coordinates:

Ir1	0.0700006699	-0.6177493485	-0.0000192679
O2	1.5656269736	-0.5228717847	1.3863121574
C3	1.3128091234	-0.5348548579	2.6380939154
C4	0.0729441886	-0.6519406755	3.2746916964
C5	-1.1612550993	-0.8156507479	2.6374755527
O6	-1.4094535049	-0.8600852400	1.3854551553
H7	-2.0463599643	-0.9374660556	3.2723865405
H8	0.0714420490	-0.6410875980	4.3589573977
H9	2.2022783994	-0.4549928288	3.2735628345
O10	-1.4100598776	-0.8599478067	-1.3848596758
C11	-1.1623628188	-0.8157418486	-2.6369721822
C12	0.0715872846	-0.6521086375	-3.2747100879
C13	1.3117219086	-0.5350398133	-2.6386320492
O14	1.5650475017	-0.5227006940	-1.3869512934
H15	2.2009550095	-0.4555010385	-3.2744667117
H16	0.0696392130	-0.6414098799	-4.3589785500
H17	-2.0477198693	-0.9377147379	-3.2715061941
C18	-0.1544135053	1.3733794837	0.0000538397
C19	-1.4378646029	1.9360248241	-0.0016811631
C20	-1.5873781973	3.3255686698	-0.0017183930
C21	-0.4687618729	4.1595467167	0.0000584246
C22	0.8075505364	3.5957105507	0.0018429250
C23	0.9714556145	2.2077830708	0.0018449647
H24	1.9666976929	1.7765188098	0.0032326013
H25	1.6866682728	4.2357311667	0.0032294650

H26	-0.5905520704	5.2393502105	0.0000268149
H27	-2.5869959201	3.7536303480	-0.0031503434
H28	-2.3119866496	1.2938413281	-0.0030488099

C (HTFA)

Gas phase Energy: -869.52189986587 hartrees

Solvation Energy: -869.50794045550 hartrees

Zero Point Energy: 130.357 kcal/mol

Coordinates:

Ir1	-0.1963584177	0.0870646895	-0.2128938346
O2	1.2562363879	0.2826972169	-1.6408194052
O3	1.2273668153	0.0483112304	1.1528518139
C4	0.9304339585	-0.0920403826	2.3981962179
C5	-0.3116818202	-0.2345996808	3.0005931613
C6	-1.5469457435	-0.2669078612	2.3315489836
O7	-1.7516634413	-0.1479101773	1.0840992403
H8	-2.4500561458	-0.4123454608	2.9341194951
H9	-0.3261695890	-0.3462421898	4.0787291174
H10	1.8218201486	-0.1008302950	3.0321110747
C11	-0.4487562423	2.0829821869	-0.2353405417
C12	-1.7476774443	2.6228050180	-0.1592360139
C13	-1.9678066567	3.9964273205	-0.3013497938
C14	-0.8920103847	4.8628125440	-0.4883092571
C15	0.4068233276	4.3465462469	-0.5386449818
C16	0.6252470079	2.9756795303	-0.4151525281
H17	1.6377182713	2.5864094101	-0.4706315718
H18	1.2515861647	5.0171867899	-0.6782859884

H19	-1.0601591841	5.9320246953	-0.5864450875
H20	-2.9813517092	4.3873707761	-0.2519307310
H21	-2.5964085235	1.9663626617	0.0169585674
O22	-0.0463060977	-2.1116041078	-0.2672165726
C23	0.8518733486	-2.6751838126	-0.9533502459
C24	1.9237772432	-0.7174645686	-2.0881636288
C25	1.8030720879	-2.0751669772	-1.8026983187
H26	0.8866602620	-3.7738068552	-0.8852051948
H27	2.6948816905	-0.4299471412	-2.8126789637
H28	2.4950169016	-2.7393387632	-2.3097346028

D (HTFA)

Gas phase Energy: -1396.35940737980 hartrees

Solvation Energy: -1396.31370607364 hartrees

Zero Point Energy: 156.045 kcal/mol

Coordinates:

Ir1	0.1126250286	-0.0381944911	0.2451561074
O2	0.6325219893	-0.2927472323	2.2155491739
O3	2.0649853116	0.0029547987	-0.1538811655
C4	2.4772352895	0.1778946927	-1.3548776188
C5	1.7383186512	0.3518719861	-2.5244529124
C6	0.3410334244	0.3782657466	-2.6191068312
O7	-0.5090042482	0.2360836670	-1.6812273220
H8	-0.0994810400	0.5407105725	-3.6089567276
H9	2.2982537239	0.4895836666	-3.4424653233
H10	3.5687933393	0.1902699146	-1.4324258967
C11	-0.0019402006	-2.0560048066	0.0493737503

C12	-0.9942965236	-2.6599188583	-0.7506030757
C13	-1.1243097604	-4.0536853997	-0.8257687454
C14	-0.2529267919	-4.8755780499	-0.1172018919
C15	0.7498528715	-4.2948152337	0.6665653784
C16	0.8698885916	-2.9090091400	0.7527693134
H17	1.6430917024	-2.4756483720	1.3796699308
H18	1.4394571889	-4.9290254256	1.2190006253
H19	-0.3456089428	-5.9565389853	-0.1769014077
H20	-1.8993709327	-4.4883956915	-1.4524799485
H21	-1.6465906081	-2.0429462827	-1.3671908585
O22	0.2640340794	2.1456669223	0.4048810666
C23	0.6735185940	2.6805235371	1.4733773074
C24	0.9677484861	0.6910457914	2.9646481139
C25	1.0155215663	2.0558355572	2.6879694528
H26	0.7661534294	3.7775829331	1.4492840764
H27	1.2518033428	0.3826835393	3.9782291074
H28	1.3407384301	2.7020498519	3.4963020125
O29	-2.0507350208	-0.2678147129	0.7606606897
H30	-2.1563365410	-1.2406351983	0.6235360158
C31	-3.1705245169	0.3604766463	0.2832011310
O32	-4.1159292012	-0.2288256326	-0.1507418425
C33	-3.1006242033	1.8991611475	0.4064939623
F34	-2.4443502903	2.4134334582	-0.6381123546
F35	-4.3462098479	2.3832119511	0.4148629058
F36	-2.4890967002	2.2631609600	1.5418817687

E (HTFA)

Gas phase Energy: -1396.38247864139 hartrees

Solvation Energy: -1396.33195859682 hartrees

Zero Point Energy: 156.153 kcal/mol

Coordinates:

Ir1	0.2531276651	-1.2570951162	-0.3179093433
C2	0.4589727265	-3.2019442104	-0.9093811020
C3	0.7788543452	-5.8759484935	-1.8016329449
C4	1.3958161588	-4.0702653049	-0.3082870574
C5	-0.3157862775	-3.7204890297	-1.9673805791
C6	-0.1579111920	-5.0390862995	-2.4063701970
C7	1.5547492002	-5.3858370826	-0.7482265683
H8	2.0153913146	-3.7030203609	0.5065167408
H9	-1.0454882741	-3.0780883665	-2.4518296035
H10	-0.7665514153	-5.4081300453	-3.2283524243
H11	2.2880151382	-6.0296797014	-0.2678455856
H12	0.9037227109	-6.8993127714	-2.1447637934
H13	-1.1129744003	-3.5393928779	0.3676011484
O14	-1.4772284660	-3.6033908564	1.2910091040
C15	-0.9674591404	-2.6658223591	2.0347715563
C16	-1.3958308545	-2.7752572072	3.5105179487
O17	-0.2210701705	-1.7477981589	1.6896893797
F18	-0.8484836724	-1.8006211766	4.2328498690
F19	-2.7318847070	-2.6861601820	3.5941494209
F20	-1.0118064246	-3.9596677265	4.0076882265
C21	3.1098407435	-0.7873281358	-0.5762531157
O22	2.2134755721	-1.1658088488	0.2454159231
H23	4.1211933904	-0.7589324237	-0.1549672289

C24	-2.5069753318	-0.3174529905	-0.7498904593
O25	-1.7497243755	-1.3543787218	-0.7948925867
H26	-3.5357202340	-0.5210981807	-1.0707616946
C27	-0.9776118674	1.4741863525	0.1095481071
C28	-2.2177774983	0.9840485270	-0.3542188829
H29	-0.9526970792	2.5396679422	0.3866386670
H30	-3.0350664191	1.6958805353	-0.4026694938
O31	0.1079804587	0.8485017570	0.2539491953
C32	1.7512487699	-0.3640535938	-2.6171402976
C33	2.9566254529	-0.4117160759	-1.9166912927
H34	1.7808562418	-0.0381549117	-3.6621641985
H35	3.8519856455	-0.1212886301	-2.4546650451
O36	0.5727252719	-0.6477500904	-2.2076481981

F (HTFA)

Gas phase Energy: -1396.37807968966 hartrees

Solvation Energy: -1396.33295086200 hartrees

Zero Point Energy: 156.531 kcal/mol

Coordinates:

Ir1	0.5942386444	-1.0034074090	-0.0479356759
O2	1.9399941543	-1.3072260565	1.4950938908
C3	1.6314806792	-2.0769609466	2.4669373513
C4	0.4174511256	-2.7126320144	2.7343676646
C5	-0.7500422472	-2.6237869585	1.9627124562
O6	-0.9469074788	-1.9843470389	0.8818714798
H7	-1.6314390905	-3.1671358237	2.3235596703
H8	0.3708737761	-3.3289659987	3.6252503431

H9	2.4493306048	-2.2384711457	3.1795030939
O10	2.1346856316	-0.0092895051	-0.9554560715
C11	-1.7448568082	1.2479316666	0.1702623563
C12	-0.3249944118	1.2755134930	0.0940438078
H13	-2.3262077953	1.3630196298	-0.7384223225
H14	0.1561459708	1.5725820044	-0.8316544422
C15	-2.3675930448	1.0727524971	1.3866682654
C16	0.4347712354	1.1118188165	1.2723428189
C17	-1.6037197167	0.9244608739	2.5678269713
C18	-0.2254855315	0.9412573124	2.5176675020
H19	-2.1107432823	0.8023174753	3.5211611772
H20	0.3625157536	0.8429383391	3.4247627872
H21	-3.4519803776	1.0553574445	1.4446866508
H22	1.5063463361	1.2745791028	1.2477049141
O23	1.1477869725	-2.8355088971	-0.6978575105
C24	2.1466963814	-2.9653012674	-1.4915540419
C25	2.9665487797	-0.6248161130	-1.6907961939
C26	3.0110086913	-1.9946741675	-1.9904035882
H27	2.3174632087	-4.0036007694	-1.7941002100
H28	3.7378230097	0.0168692360	-2.1301901248
H29	3.7990111372	-2.3307819479	-2.6542297793
C30	-0.6421800339	-0.2684710586	-2.6903849558
O31	-0.7125998643	-1.0237939996	-1.6417244769
O32	0.1456830232	0.6187355486	-2.9767775847
C33	-1.8349883932	-0.5653392770	-3.6382152144
F34	-1.6534407565	-0.0069716323	-4.8422936387
F35	-2.0359204235	-1.8830898051	-3.8161018261

F36	-2.9691227826	-0.0422808672	-3.1081137094

G (HTFA)

Gas phase Energy: -1164.09252286784 hartrees

Solvation Energy: -1164.06928145717 hartrees

Zero Point Energy: 91.933 kcal/mol

Coordinates:

Ir1	0.4317905503	-1.0875088938	-0.0213275992
O2	1.9270013172	-1.1811909657	1.3946936193
C3	1.7498690659	-1.8115314881	2.4914596054
C4	0.5922091526	-2.4415204000	2.9575738333
C5	-0.6456501374	-2.4734019903	2.3051957024
O6	-0.9621666409	-1.9845666228	1.1694032105
H7	-1.4765209823	-2.9675798894	2.8204329391
H8	0.6506728707	-2.9259720515	3.9255763821
H9	2.6336700686	-1.8349968629	3.1391517332
O10	1.7454318409	-0.0478923300	-1.1713977673
O11	1.0518825982	-2.8811446929	-0.5607734739
C12	2.0661562417	-3.0022963520	-1.3490285033
C13	2.6451794865	-0.6461812434	-1.8395803644
C14	2.8555262199	-2.0303502569	-1.9400152248
H15	2.2952282672	-4.0535215351	-1.5434113591
H16	3.3162296863	0.0171971771	-2.3945294707
H17	3.6688120345	-2.3691720093	-2.5704882396
C18	-1.0505997279	-1.0365486036	-2.5548726702
O19	-1.1036809631	-0.7395172430	-1.2854786959
O20	-0.1702671727	-1.6181430962	-3.1589076228

C21	-2.3346980052	-0.5646854823	-3.2810875825
F22	-2.2578925685	-0.8033733289	-4.5963552027
F23	-3.4169382383	-1.2083263496	-2.8004852023
F24	-2.5275293798	0.7583270438	-3.1064260698

H (HTFA)

Gas phase Energy: -1164.12231254158 hartrees

Solvation Energy: -1164.08127694637 hartrees

Zero Point Energy: 92.476 kcal/mol

Coordinates:

Ir1	-0.2412940510	0.0076813317	-0.2284235200
O2	1.1814788231	0.3295337996	-1.6560994994
O3	1.2617863571	0.0824314419	1.1300012629
C4	1.0220140376	-0.0676655299	2.3774171500
C5	-0.2010043606	-0.2734466490	3.0165296242
C6	-1.4515109050	-0.3472308184	2.3904516724
O7	-1.7245892362	-0.2489442807	1.1501515052
H8	-2.3284207407	-0.5039433793	3.0284114384
H9	-0.1817562872	-0.3783080070	4.0952445113
H10	1.9207097578	-0.0170217913	3.0013323435
O11	0.0518231682	-1.9957714140	-0.1246752568
C12	0.9559160885	-2.5604553169	-0.8315838930
C13	1.8944961236	-0.6310150579	-2.0937324035
C14	1.8369808858	-1.9871126035	-1.7490166488
H15	1.0166448814	-3.6427110754	-0.6748868452
H16	2.6376533427	-0.3296472423	-2.8403141310
H17	2.5342618490	-2.6527691615	-2.2446610715

C18	-1.7248679963	1.5950652645	-1.4376195388
O19	-0.9106325914	2.0195484069	-0.5637210876
O20	-1.7757814478	0.3542999334	-1.6892839445
C21	-2.6328147831	2.5870635609	-2.1736860941
F22	-3.4171043126	1.9583903229	-3.0534543612
F23	-3.4074012491	3.2366882939	-1.2898031188
F24	-1.8846462271	3.4895905198	-2.8280457538

I (HTFA)

Gas phase Energy: -1690.95850071363 hartrees

Solvation Energy: -1690.88994989919 hartrees

Zero Point Energy: 117.135 kcal/mol

Coordinates:

Ir1	0.1441685811	0.1037356065	0.0519873036
O2	0.5942773376	-0.7364406596	1.8591571463
O3	2.1317292692	0.3161657048	-0.2400386565
C4	2.5849252257	0.8258617132	-1.3233295808
C5	1.8826788719	1.2836071209	-2.4383214336
C6	0.4915188770	1.2627777075	-2.5947736911
O7	-0.3888264189	0.8393492299	-1.7769686533
H8	0.0785400146	1.6493979839	-3.5327455663
H9	2.4667085170	1.6844954331	-3.2586038481
H10	3.6773503838	0.8943124235	-1.3448618703
O11	0.1212059337	1.9968954106	0.7415125468
C12	0.3837196816	2.2588901298	1.9656119177
C13	0.7678543665	-0.0134299268	2.8946472082
C14	0.6875128683	1.3789555043	3.0042469675

H15	0.3543351501	3.3291119126	2.1927473080
H16	1.0119280654	-0.5816798248	3.7987648077
H17	0.8755705918	1.8117681825	3.9799019390
O18	-1.9020699741	-0.3081633825	0.4413892880
H19	-1.9101264211	-1.6807805042	0.1212375927
C20	-3.0326004710	0.3032828731	0.1092934441
O21	-4.0066782453	-0.2685127876	-0.3197419768
C22	-3.0956362393	1.8263777931	0.3916988121
F23	-2.3742862364	2.5253948233	-0.5014727409
F24	-4.3609731127	2.2528003549	0.3267125405
F25	-2.6274238927	2.1070288521	1.6276193128
O26	0.3369573529	-1.8304211287	-0.7771411914
C27	-0.5099214675	-2.7399957612	-0.6933659503
O28	-1.6852167952	-2.6785033236	-0.1958718309
C29	-0.1246063625	-4.1340344123	-1.2313602998
F30	1.0497236739	-4.0978163293	-1.8639458810
F31	-0.0384187522	-4.9936799462	-0.2039895171
F32	-1.0632328499	-4.5724055419	-2.0809023366

J (HTFA)

Gas phase Energy: -948.17333624463 hartrees

Solvation Energy: -948.15026591620 hartrees

Zero Point Energy: 165.423 kcal/mol

Coordinates:

Ir1	-0.3101382620	0.0630332550	-0.1623546766
O2	-1.9844536357	-0.1053004030	-1.3529912885
O3	0.7864692165	0.2582846355	-1.9162924847

C4	2.0554188374	0.3645113438	-1.8774314529
C5	2.9028061214	0.3723411466	-0.7644713168
C6	2.5095308236	0.2675627714	0.5724767742
O7	1.3339854148	0.1645210419	1.0585238867
H8	3.3019097147	0.2761507846	1.3299616976
H9	3.9659483633	0.4631680000	-0.9570624129
H10	2.5272609243	0.4558892488	-2.8635897568
C11	-0.4451820032	2.1301680227	-0.2456779759
C12	-1.1063926370	2.7322202369	-1.3262333076
C13	-1.1133429038	4.1216012041	-1.4808885680
C14	-0.4614588123	4.9414372574	-0.5591561038
C15	0.1969788215	4.3549251175	0.5221158618
C16	0.2019152460	2.9658581187	0.6774369880
H17	0.7243825252	2.5335875744	1.5261325629
H18	0.7119950939	4.9775859869	1.2502348602
H19	-0.4659355555	6.0212001689	-0.6817492019
H20	-1.6311234019	4.5621613737	-2.3299817754
H21	-1.6170991889	2.1127149948	-2.0553876328
O22	0.2257577818	-2.0570474752	-0.4640071465
C23	-0.4436109377	-2.7619459850	-1.2712201273
C24	-2.2598268121	-1.1851193086	-1.9816137795
C25	-1.6043161890	-2.4163523584	-1.9886053539
H26	-0.0686596847	-3.7860337921	-1.4232680284
H27	-3.1597849613	-1.1046454307	-2.6037159108
H28	-2.0332898520	-3.1864215320	-2.6207651027
C29	-1.6237076916	0.5053249854	1.5621955938
C30	-1.3874629872	-0.8677951436	1.5023623906

H31	-1.0728212789	1.1278729296	2.2576701515
H32	-0.6338430743	-1.3261087186	2.1351776688
H33	-2.1253426647	-1.5399425835	1.0741619586
H34	-2.5425209743	0.9286670080	1.1707768631

K (HTFA)

Gas phase Energy: -948.16744842331 hartrees

Solvation Energy: -948.14580907723 hartrees

Zero Point Energy: 166.004 kcal/mol

Coordinates:

Ir1	-0.4747231409	0.0914632909	-0.3423317569
O2	-1.2323222728	0.2375391648	-2.2541333524
O3	1.3239358176	0.0406396806	-1.2731343601
C4	2.4081947070	-0.1098116763	-0.6127708617
C5	2.5850322939	-0.2343324591	0.7652350868
C6	1.5616140535	-0.2120772888	1.7221327730
O7	0.3107816037	-0.0689057571	1.5399559130
H8	1.8533027767	-0.3277413153	2.7731193794
H9	3.5998126835	-0.3614206126	1.1255400845
H10	3.3022144507	-0.1412079034	-1.2458532219
O11	-0.3970389409	-2.1310047711	-0.4303306927
C12	-0.6887148949	-2.7118148628	-1.5101093043
C13	-1.3660754575	-0.7977031733	-2.9977023091
C14	-1.1449104167	-2.1460279736	-2.7207678837
H15	-0.5781029009	-3.8092599556	-1.5092673182
H16	-1.7198347111	-0.5602684201	-4.0092373974
H17	-1.3361333496	-2.8381245842	-3.5346240376

C18	-0.5175582951	2.1728960701	-0.2506011128
H19	0.1949589637	2.5201799400	0.5070932369
H20	-0.2501506212	2.6018836154	-1.2211740621
C21	-1.9647588552	2.5035803988	0.1643813714
H22	-2.0593065212	3.4165357738	0.7653409629
H23	-2.6018557685	2.6185210928	-0.7195680605
C24	-3.0316101316	-1.0870832225	2.3671801931
C25	-3.1300739068	-1.0678116898	0.9905487183
C26	-2.8128923066	0.1088651967	0.2605313904
C27	-2.4033328208	1.2814272544	0.9511713436
C28	-2.3318852463	1.2394962670	2.3592494569
C29	-2.6445233480	0.0815538539	3.0507018081
H30	-3.2621594946	-1.9910455567	2.9227472893
H31	-3.4592334083	-1.9495954721	0.4493595533
H32	-3.1107879665	0.1817108516	-0.7805498498
H33	-2.0195121191	2.1295138148	2.8981085858
H34	-2.5854069120	0.0726390793	4.1360619991

TS1 (HTFA)

Gas phase Energy: -869.51917202663 hartrees

Solvation Energy: -869.50229487639 hartrees

Zero Point Energy: 130.035 kcal/mol

Coordinates:

Ir1	-0.1061301945	0.0292477727	0.0140514137
O2	-0.1854233512	-0.0121373416	2.0627733823
O3	1.8634607994	-0.2330759716	0.1093179262
C4	2.5695957780	-0.3324232892	-0.9599876265

C5	2.1678309829	-0.2808350654	-2.2898599161
C6	0.8533774540	-0.0617680877	-2.7316848500
O7	-0.1866078568	0.1055369042	-2.0205937329
H8	0.6804354774	-0.0071316168	-3.8120759182
H9	2.9376601413	-0.3909720329	-3.0448313085
H10	3.6339195515	-0.4614134583	-0.7420243074
C11	-0.2150814459	-1.9911819024	-0.0272457277
C12	-1.1144987131	-2.6105793108	-0.9115094543
C13	-1.2986053024	-3.9974626758	-0.8918985939
C14	-0.5760475239	-4.7906265018	0.0013357722
C15	0.3307550177	-4.1857185932	0.8757985685
C16	0.5131312469	-2.8001485989	0.8593867735
H17	1.2142796278	-2.3422092749	1.5507781696
H18	0.8975301788	-4.7933597386	1.5773630426
H19	-0.7156913280	-5.8681167979	0.0144158348
H20	-2.0040855669	-4.4544258518	-1.5816168491
H21	-1.6754575254	-2.0100762664	-1.6238811905
O22	-0.7796048330	2.1022095495	0.0137260824
C23	-0.9780877241	2.7483568558	1.0922624914
C24	-0.4512319940	1.0030006676	2.7905825301
C25	-0.8084083919	2.3004830161	2.4090802440
H26	-1.3312734628	3.7819238927	0.9639229422
H27	-0.4018660837	0.7947471142	3.8658589369
H28	-1.0105162706	3.0078651130	3.2060741049

TS2 (HTFA)

Gas phase Energy: -1396.36549221748 hartrees

Solvation Energy: -1396.31614781369 hartrees

Zero Point Energy: 152.853 kcal/mol

Coordinates:

Ir1	0.0983231307	-1.3147552629	-0.1766819867
C2	0.2404121398	-3.4236763529	-0.6978902376
C3	1.0583095238	-5.5959699489	-2.3069795575
C4	1.4308744143	-4.1403214711	-0.4195578120
C5	-0.5332988667	-3.8517985488	-1.8040865826
C6	-0.1315105160	-4.9224527359	-2.5971246498
C7	1.8371058038	-5.2086426705	-1.2122595726
H8	2.0254577504	-3.8543869297	0.4433674515
H9	-1.4559082447	-3.3259072117	-2.0274280403
H10	-0.7387198016	-5.2328947334	-3.4430988446
H11	2.7537622326	-5.7439527799	-0.9800401153
H12	1.3739356022	-6.4307384757	-2.9275758282
H13	-0.4654102097	-3.4091670923	0.4122366231
O14	-1.0618353408	-3.6187619711	1.6060098102
C15	-0.9445724878	-2.5471171430	2.2465989735
C16	-1.4408122216	-2.5600413569	3.7078998234
O17	-0.4666246899	-1.4564262026	1.8262071377
F18	-1.1963985708	-1.4032207587	4.3314016543
F19	-2.7670703501	-2.7828375737	3.7283211484
F20	-0.8352103030	-3.5479921645	4.3873843997
C21	2.9884810250	-0.9918104586	-0.3649808990
O22	2.0490336419	-1.2741106118	0.4482794225
H23	3.9812017359	-0.9506165200	0.0982721223
C24	-2.5641469886	-0.2688925046	-0.7803976164

O25	-1.8791656506	-1.3470033042	-0.7208524601
H26	-3.6019763422	-0.4255126775	-1.0963536590
C27	-0.9003710718	1.4561227897	-0.0801291989
C28	-2.1729360164	1.0404694209	-0.4995582800
H29	-0.7644762689	2.5302792438	0.1010481744
H30	-2.9274445820	1.8107516426	-0.6135690838
O31	0.1385988663	0.7551046997	0.1251501522
C32	1.7407011888	-0.7399204803	-2.5055156126
C33	2.9092828992	-0.7428122046	-1.7398310780
H34	1.8386474856	-0.5272927734	-3.5762100897
H35	3.8375918803	-0.5265995852	-2.2564957140
O36	0.5381062884	-0.9502688670	-2.1331481179

TS3 (HTFA)

Gas Phase Energy: -948.10254973374 hartrees

Solvation Energy: -948.11017775328 hartrees

Zero Point Energy: 164.537 kcal/mol

Coordinates:

Ir1	-.0179673153	.0603133507	.0114309977
O2	-.0758930265	.0346857438	2.0697719582
O3	2.1444722267	-.2091755006	.1243285837
C4	2.8372676698	-.1811490654	-.9300059438
C5	2.4091937648	.0036332836	-2.2612659744
C6	1.0974517512	.1559963757	-2.7035070352
O7	-.0007724021	.1492244331	-2.0437844606
H8	.9529715708	.2855598521	-3.7834591780
H9	3.1811912316	.0208616011	-3.0233886802

H10	3.9205952719	-.3173245912	-.7870147447
C11	-.3422212543	-2.1170318833	-.0238085169
C12	.0618791115	-2.8119843248	1.1372313724
C13	.6185964193	-4.0866269832	1.0549837956
C14	.7712476326	-4.7098955126	-.1872002237
C15	.3581540173	-4.0473112516	-1.3490379850
C16	-.1990255679	-2.7748253581	-1.2668876894
H17	-.5354543549	-2.2725169613	-2.1682595285
H18	.4656730408	-4.5274162307	-2.3180219589
H19	1.2000484338	-5.7061660271	-.2498770701
H20	.9361313829	-4.5937878725	1.9621181057
H21	-.0465763759	-2.3286005503	2.1021502665
O22	.4840109963	2.0695404126	-.0867250349
C23	.6296752114	2.7640000170	.9675538104
C24	.1785258270	1.0828278602	2.7528268026
C25	.5034913376	2.3653642147	2.3060036468
H26	.8869704908	3.8148296697	.7823948326
H27	.1229284364	.9301502945	3.8374025058
H28	.6759149180	3.1213441533	3.0641340064
C29	-2.0219520904	-1.2516270304	.1489970272
C30	-2.0827809139	.2013052222	-.0335885828
H31	-2.4804932520	-1.8619762692	-.6225842431
H32	-2.4461800454	.5504636942	-.9997433307
H33	-2.4773919748	.7702980183	.8088481216
H34	-2.2407690250	-1.6067214348	1.1516316428

(1) [Ir(μ-acac-O,O,C^3)-(acac-O,O)(acac-C^3)]$_2$ was originally prepared in: Bennett, M. A.; Mitchell, T. R. B. *Inorg. Chem.* **1976**, *15*, 2936. The complex (acac-O,O)$_2$Ir(acac-C^3)(H_2O) was reported in reference 8a. The complex (acac-O,O)$_2$Ir(acac-C^3)(Pyr) was prepared in reference 8a.

(2) For the Microsoft Excel deconvolution tables see the supporting information of: Young, K. J. H.; Meier, S. K.; Gonzales, J. M.; Oxgaard, J.; Goddard, W. A. III; Periana, R. A. *Organometallics* **2006**, *25*, 4734.